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Supplementary Information (ESI): Error-consistent segmented contracted all-electron relativistic basis sets of double- and triple-zeta quality for NMR shielding constants

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Contents

1 Grids for numerical integration of the exchange-correlation potential

Relativistic effects lead to a spatial contraction of the s and p type orbitals and thus of the density. In many quantum chemical program packages, the grids for numerical integration were designed in non-relativistic calculations or with ECPs, which lead to an effective potential in the Schrödinger equation. Chemical properties, which focus on the valence shells, are well described by these methods, but for the NMR shielding tensor, which deals with the density in the core region, matters may be different. We discuss the effect of the number of radial points denoted by the grid size on relativistic all-electron approaches.

The error of the integration grids for total energies is assessed by DFT calculations of halogen atoms and compounds employing the scalar X2C Hamiltonian and the finite nucleus model at the x2c-TZVPall[1]/BP86[2,3] level of theory. All calculations were done with the X2C implementation[4,5] in TURBOMOLE.[6–8] An SCF convergence threshold of $10^{-9}E_\mathrm{h}$ was applied. The largest grid of Ref. 9 (grid 7) served as reference to measure the error. The results are shown in Tab. 1. A drastic increase of the error from Br to I is found for grid 3. A similar picture is revealed for grid 5. The errors of the molecules are in rather good agreement with the errors of the atom. Thus, it is sufficient to consider the atoms in order to improve the grids. Hence, noble gas atoms are studied and the energy is calculated with different numbers of radial grid points as displayed in Fig. 1. The energy is rapidly changing or oscillating with a small number of points in all atoms. The oscillations are damped with increasing number of points. For the heavier elements more grid points are needed.

Previously,[9] only 30 radial points were added for Ba-Rn compared to H. This is still in the oscillating region, where the energy is not converged. Moreover, the errors are not well balanced within the row as the energy of Ba will converge with less grid points than that of Rn. Based on these considerations, tailored grids for relativistic all-electron calculations (indicated by the appendix "a") are obtained by determining the number of radial grid points, r, for an atom based on the atom number, Z, according to

$$r = 20 + 5 \cdot (n-1) + Z, \tag{1}$$

where n is a parameter describing the radial grid for the Gauss-Chebyshev method. For the grids 1-5, n is given by 1,2,3,6,8. The resulting number of grid points for the studied elements is given in Tab. 2. This leads to significantly smaller errors as shown in the last three columns of Tab. 1. Thus, we suggest to use at least grid 3a in all-electron relativistic calculations. However, the effect on the NMR shieldings in the present work is rather small.

Table 1 Errors in the energy per atom in μE_h with respect to grid size 7 (largest grid available) using the X2C Hamiltonian and the finite nucleus model at the BP86/x2c-TZVPall level of theory. An SCF convergence threshold of $10^{-9}E_\mathrm{h}$ was applied. The newly developed grids feature the appendix "a".

	Grid 1	Grid 3	Grid 5	Grid 1a	Grid 3a	Grid 5a
H	−1.46	−0.15	0.00	1.46	0.15	0.00
F	−108.55	−8.86	−0.06	−5.02	−1.23	−0.03
Cl	−445.77	−12.06	−0.22	−32.01	−0.63	0.37
Br	1377.92	−209.22	−11.16	−146.80	10.83	−0.44
I	15260.23	−4557.04	44.15	514.96	−278.77	−26.25
At	53783.82	22045.85	4701.81	−2203.54	−0.01	−303.01
H_2	−15.62	−0.04	0.00	−13.35	0.04	0.00
F_2	19.63	−6.64	0.14	8.64	−3.38	−0.01
Cl_2	−170.32	−21.66	−1.77	45.01	−1.25	0.28
Br_2	2127.48	−205.83	−17.68	101.91	5.34	−0.80
I_2	15901.49	−4630.95	54.70	855.20	−292.81	−21.10
At_2	54570.64	22045.09	4719.55	−1945.71	−3.56	−296.00
HF	149.15	−6.45	−0.03	29.88	−0.60	−0.03
HCl	−198.18	−6.55	−0.13	−10.06	−0.39	0.19
HBr	658.40	−104.30	−5.57	−60.59	5.16	−0.22
HI	7632.64	−2277.93	22.06	272.45	−138.98	−13.13
HAt	26943.45	11022.17	2350.93	−1079.49	0.58	−151.50
FCl	−147.16	4.92	−0.18	15.28	3.47	0.25
FBr	502.43	−109.53	−4.58	−181.61	10.01	−0.11
FI	6961.70	−2279.38	26.52	−54.61	−139.59	−12.69
FAt	25570.29	11040.42	2362.01	−1683.62	−8.48	−149.91

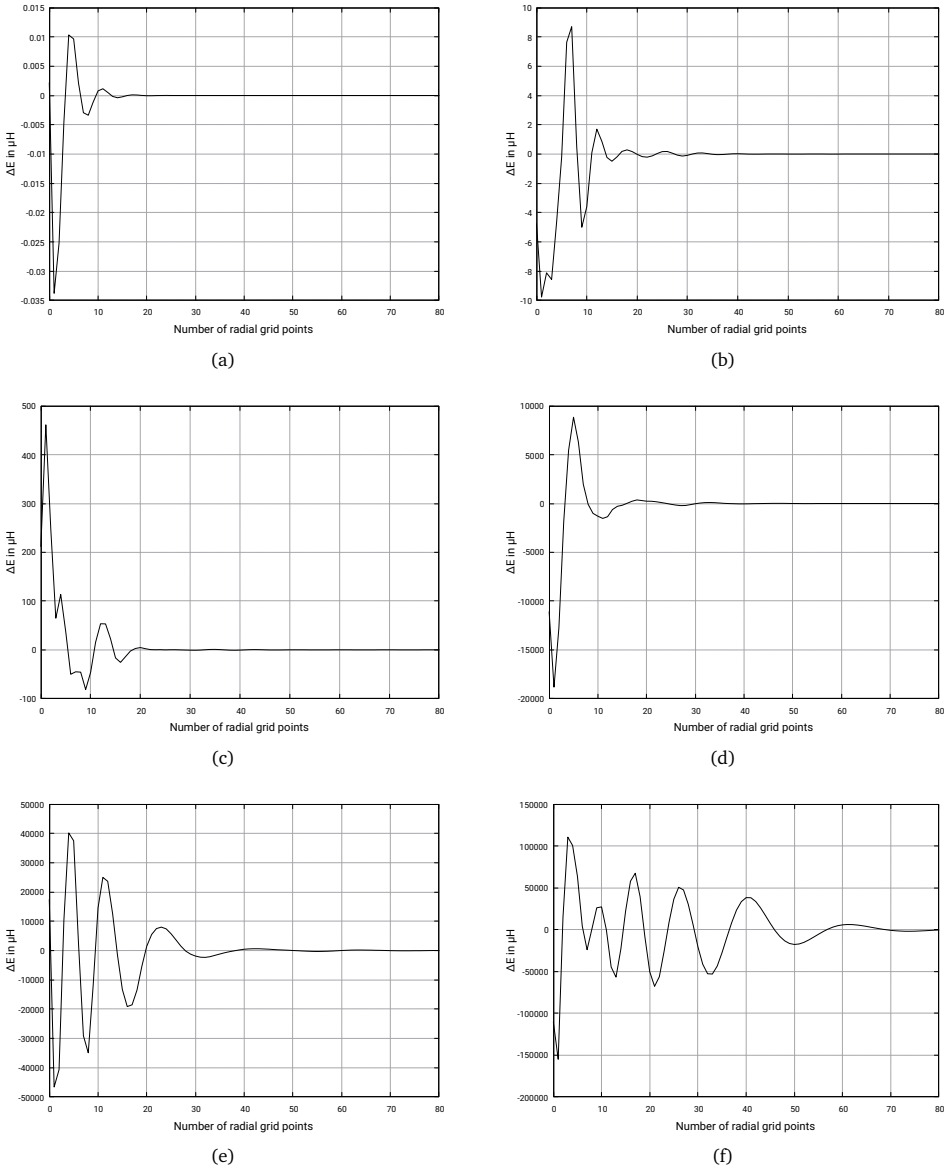

Fig. 1 Total energy difference (in μE_h, here denoted as μH) as a function of the added radial grid points for the noble gases He (a), Ne (b), Ar (c), Kr (d), Xe (e) and Rn (f). The energy difference is calculated with respect to the energy at 150 radial grid points. Zero grid points denote the number of grid points used for hydrogen (grid 3). According to Ref. 9, 5 grid points are added for Ne, 10 for Ar, 20 for Kr, 25 for Xe and 30 for Rn. For details see main text.

Table 2 Number of radial grids points for the elements H, F, Cl, Br, I and At.

	Grid 1	Grid 3	Grid 5	Grid 1a	Grid 3a	Grid 5a
H	20	30	55	20	30	55
F	25	35	60	29	39	64
Cl	30	40	65	37	47	72
Br	40	50	75	55	65	90
I	45	55	80	73	83	108
At	50	60	90	105	115	140

2 Cartesian coordinates of the molecules of the test set

Cartesian coordinates are given in the TURBOMOLE format in atomic units. Structures were collected in Ref. 10 and 11, and are given in alphabetical order herein.

Ag_2

```
  0.00000000000000      0.00000000000000     -2.43284975341900      ag
  0.00000000000000      0.00000000000000      2.43284975341900      ag
```

AgCl

```
  0.00000000000000      0.00000000000000     -2.17427221124677      ag
  0.00000000000000      0.00000000000000      2.17427221124677      cl
```

Al_2O_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      o
  0.00000000000000      0.00000000000000     -3.20592451951933      al
  0.00000000000000      0.00000000000000      3.20592451951933      al
  0.00000000000000      0.00000000000000     -6.26442328261665      o
  0.00000000000000      0.00000000000000      6.26442328261665      o
```

Al_2S_3

```
  0.00000000000000      0.00000000000000      3.16034259123655      s
 -6.05680384209421      0.00000000000000     -2.01213979070925      s
  6.05680384209421      0.00000000000000     -2.01213979070925      s
 -3.12156733278024      0.00000000000000      0.43196849509098      al
  3.12156733278024      0.00000000000000      0.43196849509098      al
```

$AlCl_3$

```
  0.00000000000000      0.00000000000000      0.00000000000000      al
  1.98010837147193     -3.42964830388186      0.00000000000000      cl
  1.98010837147193      3.42964830388186      0.00000000000000      cl
 -3.96021674294387      0.00000000000000      0.00000000000000      cl
```

AlF_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      al
  1.56643211516439     -2.71314001007231      0.00000000000000      f
  1.56643211516439      2.71314001007231      0.00000000000000      f
 -3.13286423032878      0.00000000000000      0.00000000000000      f
```

AlH_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      al
  1.51111027824900     -2.61731977776682      0.00000000000000      h
  1.51111027824900      2.61731977776682      0.00000000000000      h
 -3.02222055649801      0.00000000000000      0.00000000000000      h
```

Ar_2

```
  0.00000000000000      0.00000000000000     -3.86613649772465      ar
  0.00000000000000      0.00000000000000      3.86613649772465      ar
```

As_4

```
  1.64900717955662     -1.64900717955662      1.64900717955662      as
 -1.64900717955662      1.64900717955662      1.64900717955662      as
 -1.64900717955662     -1.64900717955662     -1.64900717955662      as
  1.64900717955662      1.64900717955662     -1.64900717955662      as
```

As_4S_4

-1.41083883866857	-1.41083883866857	4.46081971940384	s
1.41083883866857	1.41083883866857	4.46081971940384	s
-1.41083883866857	1.41083883866857	-4.46081971940384	s
1.41083883866857	-1.41083883866857	-4.46081971940384	s
0.00000000000000	3.30253054743472	0.00000000000000	as
3.30253054743472	0.00000000000000	0.00000000000000	as
0.00000000000000	-3.30253054743472	0.00000000000000	as
-3.30253054743472	0.00000000000000	0.00000000000000	as

$AsCl_3$

0.00000000000000	0.00000000000000	1.45363897308538	as
-1.85326772975506	3.20995386796359	-0.48454632436179	cl
-1.85326772975506	-3.20995386796359	-0.48454632436179	cl
3.70653545951011	0.00000000000000	-0.48454632436179	cl

AsH_3

0.00000000000000	0.00000000000000	1.23244998693740	as
-1.20159017904000	2.08121523997307	-0.41081666231247	h
-1.20159017904000	-2.08121523997307	-0.41081666231247	h
2.40318035808001	0.00000000000000	-0.41081666231247	h

At_2

0.00000000000000	0.00000000000000	-2.76898695483805	at
0.00000000000000	0.00000000000000	2.76898695483805	at

AtCl

0.00000000000000	0.00000000000000	-2.37077509436909	at
0.00000000000000	0.00000000000000	2.37077509436909	cl

AtF_3

-0.03520070639137	-0.00000061243046	0.00000000000000	at
-1.96270309041480	3.50724350882721	0.00000000000000	f
-1.96259307505300	-3.50730822874416	0.00000000000000	f
3.96049687185918	0.00006533234741	0.00000000000000	f

Au_2

0.00000000000000	0.00000000000000	-2.42327065240856	au
0.00000000000000	0.00000000000000	2.42327065240856	au

AuCl

0.00000000000000	0.00000000000000	-2.15000661513040	au
0.00000000000000	0.00000000000000	2.15000661513040	cl

B_2H_6

0.00000000000000	0.00000000000000	1.68149280660034	b
0.00000000000000	0.00000000000000	-1.68149280660034	b
0.00000000000000	-1.88412562931544	0.00000000000000	h
0.00000000000000	1.88412562931544	0.00000000000000	h
1.99832414844106	0.00000000000000	2.79335654905377	h
-1.99832414844106	0.00000000000000	2.79335654905377	h
-1.99832414844106	0.00000000000000	-2.79335654905377	h
1.99832414844106	0.00000000000000	-2.79335654905377	h

$B_3N_3H_6$

2.75503008971104	-0.00000323939483	0.00000000000000	b
1.33708167162979	2.31531468226869	0.00000000000000	n
-1.37762869492974	2.38537342180479	0.00000000000000	b
-2.67435276602476	0.00000211824938	0.00000000000000	n
-1.37764337777651	-2.38537456910514	0.00000000000000	b
1.33706851342589	-2.31531512981732	0.00000000000000	n
5.05300245977585	-0.00000804976266	0.00000000000000	h
2.30183999853162	3.98629277576524	0.00000000000000	h
-2.52609075956054	4.37610354836293	0.00000000000000	h
-4.60403920406282	0.00000416958359	0.00000000000000	h
-2.52610296250991	-4.37610284086748	0.00000000000000	h
2.30183503179008	-3.98628688708722	0.00000000000000	h

B_4H_4

1.13513007545606	1.13512970003633	1.13512888659479	b
-1.13512170839976	1.13512235099020	-1.13512294487928	b
-1.13512831829025	-1.13512872380334	1.13512812346088	b
1.13513271243326	-1.13513209595804	-1.13513301541142	b
2.45171101991862	2.45170873428443	2.45170917853944	h
-2.45171753891449	2.45171830786967	-2.45171888582538	h
-2.45170898165818	-2.45171133452650	2.45171018828927	h
2.45170273945477	-2.45170693889277	-2.45170153076831	h

Ba_4

2.98686049110414	-2.98686049110414	2.98686049110414	ba
-2.98686049110414	2.98686049110414	2.98686049110414	ba
-2.98686049110414	-2.98686049110414	-2.98686049110414	ba
2.98686049110414	2.98686049110414	-2.98686049110414	ba

BaF_2

0.00000000000000	0.00000000000000	1.55847796152849	ba
3.50406263138391	0.00000000000000	-0.77923898076424	f
-3.50406263138391	0.00000000000000	-0.77923898076424	f

BaH_2

0.00000000000000	0.00000000000000	1.68536306424487	ba
3.48553102731125	0.00000000000000	-0.84268153212243	h
-3.48553102731125	0.00000000000000	-0.84268153212243	h

BaO

0.00000000000000	0.00000000000000	-1.92962468481039	ba
0.00000000000000	0.00000000000000	1.92962468481039	o

BaS

0.00000000000000	0.00000000000000	-2.42999531404145	ba
0.00000000000000	0.00000000000000	2.42999531404145	s

Be_2F_4

-2.13361594547065	0.00000000000000	0.00000000000000	be
2.13361594547065	0.00000000000000	0.00000000000000	be
0.00000000000000	2.13211302712278	0.00000000000000	f
0.00000000000000	-2.13211302712278	0.00000000000000	f
-4.78939030299712	0.00000000000000	0.00000000000000	f
4.78939030299712	0.00000000000000	0.00000000000000	f

Be_2H_4

```
  0.00000000000000      0.00000000000000     -1.92929449970282      be
  0.00000000000000      0.00000000000000      1.92931071700141      be
  2.05284948165387      0.00000000000000     -0.00000554462538      h
 -2.05284948165387      0.00000000000000     -0.00000554462538      h
  0.00000000000000      0.00000000000000     -4.46632923721534      h
  0.00000000000000      0.00000000000000      4.46632410916751      h
```

Be_4

```
  1.98239336244068     -1.40175406475758      0.00000000000000      be
 -1.98240276048822     -1.40176820517744      0.00000000000000      be
  0.00000469902377      1.40176113496751     -1.98238088228083      be
  0.00000469902377      1.40176113496751      1.98238088228083      be
```

BeC_2H_6

```
  0.00000000000000      0.00000000000000      0.00000000000000      be
 -0.00020044556495      3.18689981828802      0.00000000000000      c
  0.00020044556495     -3.18689981828802      0.00000000000000      c
  1.94277443489397      3.99483630431448      0.00000000000000      h
  0.97131508976867     -3.99480784611534     -1.68303202724579      h
 -0.97131508976866      3.99480784611534     -1.68303202724579      h
 -1.94277443489397     -3.99483630431448      0.00000000000000      h
 -0.97131508976866      3.99480784611534      1.68303202724579      h
  0.97131508976867     -3.99480784611534      1.68303202724579      h
```

$BeF_2O_2H_4$

```
 -0.00000032363640     -0.00000008566633     -0.88438717282531      be
  0.00000013544101     -2.55923932656878     -2.01794116529110      f
 -0.00000415512240      2.55924102532360     -2.01793952586888      f
  2.70021194774609     -0.00000008523155      1.18317601953195      o
 -2.70021065005859      0.00000715003053      1.18318161817594      o
  3.67189018000387      1.47880857364976      0.63847717253928      h
 -3.67189013209522     -1.47881214872542      0.63847438690258      h
  3.67189002508221     -1.47880764617565      0.63847412415729      h
 -3.67188702736059      1.47880254336382      0.63848454267826      h
```

BeH_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      be
  0.00000000000000      0.00000000000000      2.54057183216976      h
  0.00000000000000      0.00000000000000     -2.54057183216976      h
```

BeS

```
  0.00000000000000      0.00000000000000     -1.67244267945864      be
  0.00000000000000      0.00000000000000      1.67244267945864      s
```

BF_3

```
  0.00057162011753      0.00000112131525      0.00000000000000      b
  2.50269790165942      0.00000463627076      0.00000000000000      f
 -1.25162960237501      2.16558024460409      0.00000000000000      f
 -1.25163991940193     -2.16558600219009      0.00000000000000      f
```

BH_3

```
  0.00000000000000      0.00000000000000     -0.00001716605107      b
  0.00000000000000      0.00000000000000      2.29252379962527      h
  1.98536152775083      0.00000000000000     -1.14625331603055      h
 -1.98536152775083      0.00000000000000     -1.14625331603055      h
```

BH_3CO

```
 -0.00003267004886      1.01111329216265      0.00000000000000      b
  2.24066059731720      1.62213805210289      0.00000000000000      h
 -1.12023754948246      1.62311914581523      1.94044267338909      h
 -1.12023754948246      1.62311914581523     -1.94044267338909      h
 -0.00018198607045     -1.85414688329676      0.00000000000000      c
  0.00002915776702     -4.02534275259922      0.00000000000000      o
```

BH_3NH_3

-0.00005391609667	-0.00000006055366	1.59755328544083	b
0.00003677556503	-0.00000004984535	-1.51922811870669	n
-1.12198704238829	1.94345823821240	2.21019712023369	h
-1.81066670598354	-0.00000007552669	-2.23620407950898	h
-1.12200568324154	-1.94345788468772	2.21023739863948	h
0.90537147089552	-1.56819423165877	-2.23633381411281	h
2.24393364900982	-0.00000003812768	2.21011203996588	h
0.90537145223968	1.56819410218746	-2.23633383195137	h

BiF_3

0.00000000000000	0.00000000000000	1.46232798160630	bi
1.63662897536318	-2.83472453846842	-0.48744266053543	f
1.63662897536318	2.83472453846842	-0.48744266053543	f
-3.27325795072636	0.00000000000000	-0.48744266053543	f

BiH_3

0.00000000000000	0.00000000000000	1.47386771700502	bi
1.40843659350503	-2.43948373918995	-0.49128923900167	h
1.40843659350503	2.43948373918995	-0.49128923900167	h
-2.81687318701006	0.00000000000000	-0.49128923900167	h

Br_2

0.00000000000000	0.00000000000000	-2.20336345967580	br
0.00000000000000	0.00000000000000	2.20336345967580	br

BrCl

0.00000000000000	0.00000000000000	-2.07645102410186	br
0.00000000000000	0.00000000000000	2.07645102410186	cl

C_2H_2

0.00000000000000	0.00000000000000	1.15246217269357	c
0.00000000000000	0.00000000000000	-1.15237758930046	c
0.00000000000000	0.00000000000000	3.19592252631204	h
0.00000000000000	0.00000000000000	-3.19600710970514	h

C_2H_3N

1.88736354706722	-0.38569072500046	0.00000000000000	n
-0.71824807664584	-0.19471094953120	-1.22023694426924	c
-0.71824807664584	-0.19471094953120	1.22023694426924	c
2.62906670020725	1.44277863614961	0.00000000000000	h
-1.53996704699139	-0.33383300604337	-3.10934257471802	h
-1.53996704699139	-0.33383300604337	3.10934257471802	h

C_2H_4

-0.00000595240645	-1.26733455985489	0.00000000000000	c
-0.00001103692376	1.26733990808114	0.00000000000000	c
1.77139591530185	-2.36353680346697	0.00000000000000	h
-1.77135302848125	-2.36354228611354	0.00000000000000	h
1.77143988920888	2.36354006871598	0.00000000000000	h
-1.77146578669927	2.36353367263826	0.00000000000000	h

C_2H_6

-0.00004769714133	0.00000349348608	1.44636083928208	c
0.00000804691144	0.00000483284596	-1.44638600827020	c
0.00000507341384	1.94903094277111	2.21977150357274	h
-1.68811904618790	0.97442869763498	-2.21944595476968	h
-1.68812247614916	-0.97443046693153	2.21943006405761	h
0.00000720306362	-1.94903334377391	-2.21978760781604	h
1.68813497191566	-0.97443316442446	2.21950311354087	h
1.68813392417380	0.97442900839179	-2.21944594959735	h

C_4H_4

0.99384594007199	0.99384464702096	0.99383622488147	c
-0.99383778119390	0.99384857359297	-0.99384786547507	c
-0.99383837692231	-0.99383758446481	0.99383909184982	c
0.99384393287549	-0.99383406319256	-0.99384192088452	c
2.18053060627208	2.18052818251503	2.18055255481919	h
-2.18053790501712	2.18055083059018	-2.18055040079725	h
-2.18053792505281	-2.18054059788475	2.18054096602118	h
2.18053150896658	-2.18055998817700	-2.18052865041484	h

C_6H_6

2.65617581771435	-0.00001755566762	0.00000000000000	c
1.32809320450038	2.30036580039517	0.00000000000000	c
-1.32814289699474	2.30032454944275	0.00000000000000	c
-2.65616474222357	-0.00002947176151	0.00000000000000	c
-1.32814664832257	-2.30031670879657	0.00000000000000	c
1.32804572900546	-2.30030596170580	0.00000000000000	c
4.73697603254869	-0.00001003497658	0.00000000000000	h
2.36858554692983	4.10225225927773	0.00000000000000	h
-2.36858598921966	4.10217914017551	0.00000000000000	h
-4.73684964271648	-0.00000987434447	0.00000000000000	h
-2.36856197133617	-4.10217066208403	0.00000000000000	h
2.36857556011450	-4.10226147995460	0.00000000000000	h

Ca_4

2.85158388323171	2.85158388323171	2.85158388323171	ca
-2.85158388323171	2.85158388323171	-2.85158388323171	ca
-2.85158388323171	-2.85158388323171	2.85158388323171	ca
2.85158388323171	-2.85158388323171	-2.85158388323171	ca

$CaCl_2$

0.00000000000000	0.00000000000000	0.00000000000000	ca
0.00000000000000	0.00000000000000	-4.87191849109726	cl
0.00000000000000	0.00000000000000	4.87191849109726	cl

Cs_2

0.00000000000000	0.00000000000000	4.46659514524658	cs
0.00000000000000	0.00000000000000	-4.46659514524658	cs

CaF_2

0.00000000000000	0.00000000000000	0.00000000000000	ca
0.00000000000000	0.00000000000000	-3.97143043764854	f
0.00000000000000	0.00000000000000	3.97143043764854	f

CaH_2

0.00000000000000	0.00000000000000	0.00000000000000	ca
0.00000000000000	0.00000000000000	4.04362377931292	h
0.00000000000000	0.00000000000000	-4.04362377931292	h

Cd_2

0.00000000000000	0.00000000000000	-3.50015172615381	cd
0.00000000000000	0.00000000000000	3.50015172615381	cd

Cd_2Cl_2

0.00000000000000	0.00000000000000	-2.47695311983738	cd
0.00000000000000	0.00000000000000	2.47695311983738	cd
0.00000000000000	0.00000000000000	-6.88014958103161	cl
0.00000000000000	0.00000000000000	6.88014958103161	cl

CdF_2

0.00000000000000	0.00000000000000	0.00000000000000	cd
0.00000000000000	0.00000000000000	3.65399698977701	f
0.00000000000000	0.00000000000000	-3.65399698977701	f

$Cd(CH_3)_2$

0.00000000000000	0.00000000000000	0.00000000000000	cd
4.03002561689173	0.00000000000000	0.00000000000000	c
-4.03002561689173	0.00000000000000	0.00000000000000	c
4.77052733051605	-1.70350166495880	-0.98351714482894	h
4.77052733051605	0.00000000000000	1.96703428965788	h
4.77052733051605	1.70350166495880	-0.98351714482894	h
-4.77052733051605	1.70350166495880	-0.98351714482894	h
-4.77052733051605	0.00000000000000	1.96703428965788	h
-4.77052733051605	-1.70350166495880	-0.98351714482894	h

CF_4

0.00000072798427	-0.00000084127378	0.00000134823270	c
1.45612263947210	1.45612426874410	1.45612670863342	f
-1.45612382956586	1.45612744820956	-1.45611634123477	f
-1.45611302972194	-1.45611774949082	1.45611910063923	f
1.45611349183143	-1.45613312618904	-1.45613081627060	f

CH_2O_2

-0.00257696271985	-0.00029911539700	0.43566389538811	c
0.91809787651456	1.10119962920547	-1.77030267443462	o
-0.89638419996679	-1.09806893130047	-1.78331456460493	o
1.35822195950510	-1.13175262110298	1.56631140453024	h
-1.37735867333304	1.12892103859498	1.55164193912118	h

CH_2O

0.00001136906018	-0.00680178712325	0.00000000000000	c
0.00001124892632	-2.29137576741941	0.00000000000000	o
-1.79950764336418	1.14910699652609	0.00000000000000	h
1.79948502537768	1.14907055801657	0.00000000000000	h

CH_3N

-0.51099882579378	-1.72615900810017	0.00000000000000	n
-0.28199635256966	0.67673092847568	0.00000000000000	c
1.26548359579527	-2.55925182755683	0.00000000000000	h
1.54014071938432	1.74203610207273	0.00000000000000	h
-2.01262913681617	1.86664380510858	0.00000000000000	h

CH_4

0.00000365772543	-0.00000430204539	-0.00000303470922	c
1.20635474089927	1.20638206443483	1.20635809459961	h
-1.20637417661767	1.20636079380735	-1.20635435342573	h
-1.20635629114801	-1.20637256903187	1.20636439312342	h
1.20637206914099	-1.20636598716490	-1.20636509958807	h

Cl_2

0.00000000000000	0.00000000000000	1.94562946845339	cl
0.00000000000000	0.00000000000000	-1.94562946845339	cl

ClF_3

-0.00003067860727	-0.83736782989924	0.00000000000000	cl
-3.32968626746479	-0.75728391745932	0.00000000000000	f
3.32967523209023	-0.75719934611368	0.00000000000000	f
0.00004171398183	2.35185109347225	0.00000000000000	f

ClF

0.00000000000000	0.00000000000000	-1.58509614282258	cl
0.00000000000000	0.00000000000000	1.58509614282258	f

CO_2

0.00000000000000	0.00000000000000	0.00002806040915	c
0.00000000000000	0.00000000000000	2.21994735057408	o
0.00000000000000	0.00000000000000	-2.21997541098322	o

CO

0.00000000000000	0.00000000000000	-1.07901367410215	c
0.00000000000000	0.00000000000000	1.07901367410215	o

$Cr(CO)_6$

0.00000000000000	0.00000000000000	0.00000000000000	cr
0.00000000000000	3.59171681854581	0.00000000000000	c
0.00000000000000	0.00000000000000	3.59171681854581	c
3.59171681854581	0.00000000000000	0.00000000000000	c
0.00000000000000	0.00000000000000	-3.59171681854581	c
-3.59171681854581	0.00000000000000	0.00000000000000	c
0.00000000000000	-3.59171681854581	0.00000000000000	c
0.00000000000000	5.77973936611907	0.00000000000000	o
0.00000000000000	0.00000000000000	5.77973936611907	o
5.77973936611907	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	-5.77973936611907	o
-5.77973936611907	0.00000000000000	0.00000000000000	o
0.00000000000000	-5.77973936611907	0.00000000000000	o

CrO_3

0.00000000000000	0.00000000000000	0.00000000000000	cr
-1.50063115995876	2.59916941246959	0.00000000000000	o
-1.50063115995876	-2.59916941246959	0.00000000000000	o
3.00126231991752	0.00000000000000	0.00000000000000	o

CS_2

0.00000000000000	0.00000000000000	-0.00042370317242	c
0.00000000000000	0.00000000000000	2.96976471283164	s
0.00000000000000	0.00000000000000	-2.96934100965921	s

CsF

0.00000000000000	0.00000000000000	-2.43002010389848	f
0.00000000000000	0.00000000000000	2.43002010389848	cs

CsH

0.00000000000000	0.00000000000000	-2.51401278411792	cs
0.00000000000000	0.00000000000000	2.51401278411792	h

Cu_2

0.00000000000000	0.00000000000000	-2.07387116344728	cu
0.00000000000000	0.00000000000000	2.07387116344728	cu

Cu_2O

0.00000000000000	0.00000000000000	1.63312192704579	o
2.28854347532692	0.00000000000000	-0.81656096352289	cu
-2.28854347532692	0.00000000000000	-0.81656096352289	cu

Cu_2S

0.00000000000000	0.00000000000000	2.19080233145777	s
-2.28384138036123	0.00000000000000	-1.09540116572889	cu
2.28384138036123	0.00000000000000	-1.09540116572889	cu

CuCl

0.00000000000000	0.00000000000000	-1.95954303758138	cu
0.00000000000000	0.00000000000000	1.95954303758138	cl

CuCN

0.00000000000000	0.00000000000000	-3.01968451426437	cu
0.00000000000000	0.00000000000000	0.39611548720036	c
0.00000000000000	0.00000000000000	2.62356902706402	n

CuF

0.00000000000000	0.00000000000000	-1.64676654637877	cu
0.00000000000000	0.00000000000000	1.64676654637877	f

CuH

0.00000000000000	0.00000000000000	-1.37926640891550	cu
0.00000000000000	0.00000000000000	1.37926640891550	h

F_2

0.00000000000000	0.00000000000000	-1.33472243762606	f
0.00000000000000	0.00000000000000	1.33472243762606	f

$Fe(CO)_5$

0.00000000000000	0.00000000000000	0.00000000000000	fe
1.70357480283978	-2.95067811301262	0.00000000000000	c
1.70357480283978	2.95067811301262	0.00000000000000	c
-3.40714960567955	0.00000000000000	0.00000000000000	c
0.00000000000000	0.00000000000000	3.40816318478371	c
0.00000000000000	0.00000000000000	-3.40816318478371	c
2.79922085086665	-4.84839273530721	0.00000000000000	o
2.79922085086665	4.84839273530721	0.00000000000000	o
-5.59844170173329	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	5.59447063964439	o
0.00000000000000	0.00000000000000	-5.59447063964439	o

Ferrocene

0.00000000000000	0.00000000000000	0.00000000000000	fe
2.31561104541701	0.00000000000000	3.09927116392114	c
0.71556316539619	2.20227697394888	3.09927116392114	c
-1.87336868810470	1.36108202254167	3.09927116392114	c
-1.87336868810470	-1.36108202254167	3.09927116392114	c
0.71556316539619	-2.20227697394888	3.09927116392114	c
2.31561104541701	0.00000000000000	-3.09927116392114	c
0.71556316539619	-2.20227697394888	-3.09927116392114	c
-1.87336868810470	-1.36108202254167	-3.09927116392114	c
-1.87336868810470	1.36108202254167	-3.09927116392114	c
0.71556316539619	2.20227697394888	-3.09927116392114	c
4.38900985665904	0.00000000000000	3.08518706538327	h
1.35627863418680	4.17419642425924	3.08518706538327	h

```
 -3.55078356251632      2.57979526591049      3.08518706538327      h
 -3.55078356251632     -2.57979526591049      3.08518706538327      h
  1.35627863418680     -4.17419642425924      3.08518706538327      h
  4.38900985665904      0.00000000000000     -3.08518706538327      h
  1.35627863418680     -4.17419642425924     -3.08518706538327      h
 -3.55078356251632     -2.57979526591049     -3.08518706538327      h
 -3.55078356251632      2.57979526591049     -3.08518706538327      h
  1.35627863418680      4.17419642425924     -3.08518706538327      h
```

$GaCl_4$

```
  0.00000000000000      0.00000000000000      0.00000000000000      ga
  2.02363708334148     -3.50504224442794      0.00000000000000      cl
  2.02363708334148      3.50504224442794      0.00000000000000      cl
 -4.04727416668296      0.00000000000000      0.00000000000000      cl
```

GaCl

```
  0.00000000000000      0.00000000000000     -2.11198999351902      ga
  0.00000000000000      0.00000000000000      2.11198999351902      cl
```

GaF

```
  0.00000000000000      0.00000000000000     -1.69732010119943      ga
  0.00000000000000      0.00000000000000      1.69732010119943      f
```

GaH_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      ga
  1.49230772481659     -2.58475279990984      0.00000000000000      h
  1.49230772481659      2.58475279990984      0.00000000000000      h
 -2.98461544963317      0.00000000000000      0.00000000000000      h
```

$GeCl_4$

```
  0.00000000000000      0.00000000000000      0.00000000000000      ge
  2.34720419578646     -2.34720419578646      2.34720419578646      cl
 -2.34720419578646      2.34720419578646      2.34720419578646      cl
 -2.34720419578646     -2.34720419578646     -2.34720419578646      cl
  2.34720419578646      2.34720419578646     -2.34720419578646      cl
```

GeF_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      ge
  1.87482477759343     -1.87482477759343      1.87482477759343      f
 -1.87482477759343      1.87482477759343      1.87482477759343      f
 -1.87482477759343     -1.87482477759343     -1.87482477759343      f
  1.87482477759343      1.87482477759343     -1.87482477759343      f
```

GeH_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      ge
  1.69283500661777     -1.69283500661777      1.69283500661777      h
 -1.69283500661777      1.69283500661777      1.69283500661777      h
 -1.69283500661777     -1.69283500661777     -1.69283500661777      h
  1.69283500661777      1.69283500661777     -1.69283500661777      h
```

GeO_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      ge
  0.00000000000000      0.00000000000000      3.09562411619127      o
  0.00000000000000      0.00000000000000     -3.09562411619127      o
```

GeO

```
  0.00000000000000      0.00000000000000     -1.55696412775958      ge
  0.00000000000000      0.00000000000000      1.55696412775958      o
```

H_2

```
  0.00000000000000      0.00000000000000      0.72490772298399      h
  0.00000000000000      0.00000000000000     -0.72490772298399      h
```

H_2CO_3

-0.00000072368405	0.22080394668051	0.00000000000000	c
-0.00000085983362	2.51789433031705	0.00000000000000	o
2.06907082035747	-1.26682714026337	0.00000000000000	o
-2.06907034454166	-1.26683026979785	0.00000000000000	o
3.50618225374280	-0.10251893084200	0.00000000000000	h
-3.50618114604093	-0.10252193609435	0.00000000000000	h

H_2O_2

1.37391573291828	-0.11754325013582	0.47481512973650	o
-1.37391573291828	0.11754325013582	0.47481512973650	o
1.81764940640807	1.41027485517298	-0.47481512973649	h
-1.81764940640807	-1.41027485517298	-0.47481512973649	h

H_2O

-0.00000092153086	0.77139067871094	0.00000000000000	o
1.43408493447591	-0.38569466553748	0.00000000000000	h
-1.43408401294505	-0.38569601317346	0.00000000000000	h

H_2SO_4

-0.00001618652064	0.00000532998352	0.57726346501965	s
2.40449042802622	0.00000119792204	1.95483853136064	o
-2.40446876756433	0.00000117641825	1.95482480979171	o
-0.00000130197438	2.22843215334819	-1.58826869332215	o
-0.00000131291374	-2.22844560147121	-1.58825020322016	o
-0.00000143369034	3.83405981964557	-0.65522713489551	h
-0.00000142536279	-3.83405407584636	-0.65518077473415	h

H_3PO_4

0.00025271029759	0.00000002775195	0.18378624273833	p
2.75771513369481	0.00000046305733	-1.18697263987526	o
-1.38058842041890	2.38580178738371	-1.18704930153066	o
-1.38058701560059	-2.38580233754762	-1.18704935129008	o
0.00141162249612	0.00000008197607	3.01262148875343	o
4.05947580693281	-0.00000015128153	0.12202776723928	h
-2.02883988453177	3.51548597828379	0.12131791511576	h
-2.02883995287005	-3.51548584962367	0.12131787884917	h

HBr

0.00000000000000	0.00000000000000	-1.35667371651595	h
0.00000000000000	0.00000000000000	1.35667371651595	br

$HCBr_3$

0.00000000000000	0.00000000000000	0.22579559169999	c
0.00000000000000	0.00000000000000	2.30613641574210	h
1.76507167530612	-3.05719382063092	-0.84397733581403	br
1.76507167530612	3.05719382063092	-0.84397733581403	br
-3.53014335061225	0.00000000000000	-0.84397733581403	br

HCl

0.00000000000000	0.00000000000000	-1.22530682104886	cl
0.00000000000000	0.00000000000000	1.22530682104886	h

HCN

0.00000000000000	0.00000000000000	-2.10459881646616	h
0.00000000000000	0.00000000000000	-0.05057148541107	c
0.00000000000000	0.00000000000000	2.15517030187723	n

HCP

0.00000000000000	0.00000000000000	-2.64853987727355	p
0.00000000000000	0.00000000000000	2.35551089579161	h
0.00000000000000	0.00000000000000	0.29302898148195	c

He_2

0.00000000000000	0.00000000000000	-2.73321591412282	he
0.00000000000000	0.00000000000000	2.73321591412282	he

HF

```
  0.00000000000000      0.00000000000000      0.88143111896247      h
  0.00000000000000      0.00000000000000     -0.88143111896247      f
```

HfO_2

```
  0.00000000000000      0.00000000000000      1.37910110648005      hf
  2.72240351204331      0.00000000000000     -0.68955055324002      o
 -2.72240351204331      0.00000000000000     -0.68955055324002      o
```

HfO

```
  0.00000000000000      0.00000000000000     -1.66226332616427      hf
  0.00000000000000      0.00000000000000      1.66226332616427      o
```

Hg_2

```
  0.00000000000000      0.00000000000000     -3.56213476071695      hg
  0.00000000000000      0.00000000000000      3.56213476071695      hg
```

Hg_2Cl_2

```
 -0.00092289111444     -2.49971029372210      0.00000000000000      hg
  0.00086843425201      2.49894980264274      0.00000000000000      hg
  0.00005416705884     -6.97426742991672      0.00000000000000      cl
  0.00000028980360      6.97502792099608      0.00000000000000      cl
```

HgF_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      hg
  0.00000000000000      0.00000000000000     -3.69723523229824      f
  0.00000000000000      0.00000000000000      3.69723523229824      f
```

$Hg(CH_3)_2$

```
  0.00000000000000      0.00000000000000      0.00000000000000      hg
  0.00000000000000      0.00000000000000      4.03656130521134      c
  0.00000000000000      0.00000000000000     -4.03656130521134      c
  1.70138176612670     -0.98229322066757      4.76366724761748      h
  1.70138176612670      0.98229322066757     -4.76366724761748      h
  0.00000000000000      1.96458644133514      4.76366724761748      h
 -1.70138176612670      0.98229322066757     -4.76366724761748      h
 -1.70138176612670     -0.98229322066757      4.76366724761748      h
  0.00000000000000     -1.96458644133514     -4.76366724761748      h
```

HI

```
  0.00000000000000      0.00000000000000     -1.54901575226915      i
  0.00000000000000      0.00000000000000      1.54901575226915      h
```

HNC

```
  0.00000000000000      0.00000000000000     -2.02196172790527      h
  0.00000000000000      0.00000000000000     -0.10820520253614      n
  0.00000000000000      0.00000000000000      2.13016693044140      c
```

HNO_2

```
 -0.00005991769124      0.00467141411420      0.00000000000000      n
  0.00050822247803     -2.00908183598864      0.00000000000000      h
  2.08688969332883      1.00263775985379      0.00000000000000      o
 -2.08733799811562      1.00177266202064      0.00000000000000      o
```

HNO_3

```
 -0.84920495946036     -0.15764648097179      0.00000000000000      n
 -1.28916831029594      2.10044345874920      0.00000000000000      o
  1.78029964374549     -0.83073113266367      0.00000000000000      o
 -2.25079424696181     -1.94859046351144      0.00000000000000      o
  2.60886787297262      0.83652461839769      0.00000000000000      h
```

HNO

```
 -1.79661507816673      0.48943320881840      0.00000000000000      o
  0.47454096973458      0.69971484027459      0.00000000000000      n
  1.32207410843215     -1.18914804909299      0.00000000000000      h
```

H_2S

-0.00000891346937	1.19653856768716	0.00000000000000	s
1.84307080535555	-0.59826448731836	0.00000000000000	h
-1.84306189188618	-0.59827408036881	0.00000000000000	h

H_2S_2

1.98198459838609	-0.07543787142517	0.90366573347496	s
-1.98198459838609	0.07543787142517	0.90366573347496	s
2.42926401991953	1.72380811808687	-0.90366607995143	h
-2.42926401991953	-1.72380811808687	-0.90366607995143	h

I_2

0.00000000000000	0.00000000000000	-2.58717910006003	i
0.00000000000000	0.00000000000000	2.58717910006003	i

ICl

0.00000000000000	0.00000000000000	-2.27749291163188	i
0.00000000000000	0.00000000000000	2.27749291163189	cl

$InCl_3$

0.00000000000000	0.00000000000000	0.00000000000000	in
-2.18888514352907	3.79126028052504	0.00000000000000	cl
-2.18888514352907	-3.79126028052504	0.00000000000000	cl
4.37777028705814	0.00000000000000	0.00000000000000	cl

InCl

0.00000000000000	0.00000000000000	-2.28501380453881	in
0.00000000000000	0.00000000000000	2.28501380453881	cl

InH_3

0.00000000000000	0.00000000000000	0.00000000000000	in
-1.65719731255026	2.87034994350365	0.00000000000000	h
-1.65719731255026	-2.87034994350365	0.00000000000000	h
3.31439462510052	0.00000000000000	0.00000000000000	h

InH

0.00000000000000	0.00000000000000	-1.77323971157117	in
0.00000000000000	0.00000000000000	1.77323971157117	h

K_2

3.78265681156495	0.00000000000000	0.00000000000000	k
-3.78265681156495	0.00000000000000	0.00000000000000	k

K_2S

0.00000000000000	0.00000000000000	1.75493373992356	s
-4.68812462132366	0.00000000000000	-0.87746686996178	k
4.68812462132366	0.00000000000000	-0.87746686996178	k

K_3P

0.00000000000000	0.00000000000000	1.89749417626207	p
2.58580346543032	-4.47874298051299	-0.63249805875402	k
2.58580346543032	4.47874298051299	-0.63249805875402	k
-5.17160693086064	0.00000000000000	-0.63249805875402	k

KBr

0.00000000000000	0.00000000000000	-2.75588742538509	k
0.00000000000000	0.00000000000000	2.75588742538509	br

KCl

0.00000000000000	0.00000000000000	-2.59307106746649	k
0.00000000000000	0.00000000000000	2.59307106746649	cl

KF

0.00000000000000	0.00000000000000	-2.13462007168556	k
0.00000000000000	0.00000000000000	2.13462007168556	f

KH

0.00000000000000	0.00000000000000	-2.20252950247800	k
0.00000000000000	0.00000000000000	2.20252950247800	h

KI

0.00000000000000	0.00000000000000	-3.00693295045154	k
0.00000000000000	0.00000000000000	3.00693295045154	i

$LaCl_3$

0.00000000000000	0.00000000000000	0.96009113070341	la
2.39456067083526	-4.14750074369288	-0.32003037690110	cl
2.39456067083526	4.14750074369288	-0.32003037690110	cl
-4.78912134167051	0.00000000000000	-0.32003037690110	cl

LaF_3

0.00835382361157	-1.02117071692355	0.00000000000000	la
1.91439485833747	0.34319474197956	-3.33760883218938	f
1.91439485833747	0.34319474197956	3.33760883218938	f
-3.83714354028650	0.33478123296444	0.00000000000000	f

LaH_3

0.00000000000000	0.00000000000000	1.12917729323785	la
1.86921337577393	-3.23757253702778	-0.37639243107929	h
1.86921337577393	3.23757253702778	-0.37639243107929	h
-3.73842675154786	0.00000000000000	-0.37639243107929	h

Li_2

0.00000000000000	0.00000000000000	2.64099487417752	li
0.00000000000000	0.00000000000000	-2.64099487417752	li

Li_2O

0.00000000000000	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	3.07886917104883	li
0.00000000000000	0.00000000000000	-3.07886917104883	li

$Li_4C_4H_{12}$

1.64706365185023	-1.64706414193258	1.64706544369022	li
-1.64706403016091	1.64706609392631	1.64705887225055	li
-1.64706511498339	-1.64706283357271	-1.64706684500640	li
1.64706611886332	1.64706488898669	-1.64706698536379	li
-2.43039744530168	-2.43039421024393	2.43039371335858	c
-2.43039481981438	2.43039861558535	-2.43039404610143	c
2.43041016795889	-2.43037962486503	-2.43040830076453	c
2.43039584881608	2.43039712925517	2.43039442430495	c
-3.75314966263209	-3.75314808906104	1.42781762772074	h
-3.75315152314663	1.42782582005728	-3.75315082553213	h
3.75314761464945	-3.75315658904388	-1.42781372983920	h
3.75314887684819	1.42782119712603	3.75314726754457	h
3.75315353972696	-1.42784583286734	-3.75312947798914	h
-1.42781763382581	3.75315092168214	-3.75315637933721	h
-1.42782024327477	-3.75314815761710	3.75314688009472	h
3.75314899897099	3.75315138842044	1.42781694923781	h
1.42781612597795	-3.75315104845671	-3.75315272040008	h
-3.75315006597704	-1.42781843578250	3.75314714040825	h
1.42782002306320	3.75315047748770	3.75314651403628	h
-3.75316042760865	3.75314243091576	-1.42779552231280	h

Li_4Cl_4

2.74433107302748	-1.94051594179951	0.00000000000000	li
0.00000067632057	1.94051446095008	2.74434044508148	li
-2.74434673087586	-1.94050438549579	0.00000000000000	li
0.00000067632057	1.94051446095008	-2.74434044508148	li
3.45559531815124	2.44348827432849	0.00000000000000	cl
-0.00000377172669	-2.44349841628354	3.45558889743391	cl
-3.45557361860438	2.44349993543522	0.00000000000000	cl
-0.00000377172669	-2.44349841628354	-3.45558889743391	cl

Li_4H_4

1.70080534683096	1.70080537092335	1.70080629791783	li
-1.70080500921405	1.70080539807377	-1.70080575731674	li
-1.70080602667080	-1.70080602949547	1.70080562105870	li
1.70080538482293	-1.70080498514297	-1.70080576838347	li
-1.85949824812399	1.85949816528516	1.85949815526986	h
-1.85949848558192	-1.85949846568449	-1.85949840131317	h
1.85949821284325	-1.85949826186725	1.85949814331282	h
1.85949882509361	1.85949880790790	-1.85949829054584	h

Li_8

```
  2.74131108923626      2.74132478269676      2.74117649987501      li
 -2.74132095967384      2.74139733087893      2.74123662814823      li
 -2.74141505700265     -2.74140311587089      2.74132801066027      li
  2.74142424897969     -2.74136699425814      2.74128552508306      li
  2.74120592621730     -2.74115999255214     -2.74129238641303      li
  2.74113282151043      2.74114762466293     -2.74121705828456      li
 -2.74113063835797      2.74118015543297     -2.74125140645887      li
 -2.74120743090921     -2.74111979099044     -2.74126581261013      li
```

$LiBH_4$

```
 -0.00024869116689     -0.69457330488353      0.00000000000000      b
  0.00086758333408     -2.99344227721830      0.00000000000000      h
  1.10203755028072      0.22558430838791     -1.90940541026977      h
  1.10203755028072      0.22558430838791      1.90940541026977      h
 -2.20471760670618      0.22450989127912      0.00000000000000      h
  0.00002361397754      3.01233707404689      0.00000000000000      li
```

LiCl

```
  0.00000000000000      0.00000000000000     -1.93849439881658      li
  0.00000000000000      0.00000000000000      1.93849439881658      cl
```

LiF

```
  0.00000000000000      0.00000000000000     -1.48697136026104      li
  0.00000000000000      0.00000000000000      1.48697136026103      f
```

LiH

```
  0.00000000000000      0.00000000000000      1.54697769798700      li
  0.00000000000000      0.00000000000000     -1.54697769798700      h
```

Li_2S

```
  0.00000000000000      0.00000000000000      0.00000000000000      s
  0.00000000000000      0.00000000000000      3.94716240337943      li
  0.00000000000000      0.00000000000000     -3.94716240337943      li
```

Mg_4

```
  2.14509045506480     -2.14509045506480      2.14509045506480      mg
 -2.14509045506480      2.14509045506480      2.14509045506480      mg
 -2.14509045506480     -2.14509045506480     -2.14509045506480      mg
  2.14509045506480      2.14509045506480     -2.14509045506480      mg
```

$MgCl_2$

```
  0.00000000000000      0.00000000000000      0.00000000000000      mg
  0.00000000000000      0.00000000000000      4.14223402210192      cl
  0.00000000000000      0.00000000000000     -4.14223402210192      cl
```

MgF_2

0.00000000000000	0.00000000000000	0.00000000000000	mg
0.00000000000000	0.00000000000000	3.32239429304949	f
0.00000000000000	0.00000000000000	-3.32239429304949	f

MgH_2

0.00000000000000	0.00000000000000	0.00000000000000	mg
0.00000000000000	0.00000000000000	3.23157098894782	h
0.00000000000000	0.00000000000000	-3.23157098894782	h

Mo_2

0.00000000000000	-1.94953471197013	0.00000000000000	mo
0.00000000000000	1.94953471197013	0.00000000000000	mo

$Mo(CO)_6$

0.00000000000000	0.00000000000000	0.00000000000000	mo
0.00000000000000	3.90295652556995	0.00000000000000	c
0.00000000000000	0.00000000000000	3.90295652556995	c
3.90295652556995	0.00000000000000	0.00000000000000	c
0.00000000000000	0.00000000000000	-3.90295652556995	c
-3.90295652556995	0.00000000000000	0.00000000000000	c
0.00000000000000	-3.90295652556995	0.00000000000000	c
0.00000000000000	6.09006160839460	0.00000000000000	o
0.00000000000000	0.00000000000000	6.09006160839460	o
6.09006160839460	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	-6.09006160839460	o
-6.09006160839460	0.00000000000000	0.00000000000000	o
0.00000000000000	-6.09006160839460	0.00000000000000	o

MoO_3

0.00000000000000	0.00000000000000	-0.87497023552764	mo
-1.52984968466562	2.64977738178409	0.29165674517588	o
-1.52984968466562	-2.64977738178409	0.29165674517588	o
3.05969936933125	0.00000000000000	0.29165674517588	o

N_2

0.00000000000000	0.00000000000000	-1.05078974035833	n
0.00000000000000	0.00000000000000	1.05078974035833	n

N_2H_2

-1.17672812398851	0.92386039472759	0.00000000000000	n
1.17661864072211	0.92396010505874	0.00000000000000	n
-1.95539025873620	-0.92400022187768	0.00000000000000	h
1.95549974200260	-0.92382027790864	0.00000000000000	h

N_2H_4

1.34301342554004	0.11487732805038	0.44262664845470	n
-1.34301342554004	-0.11487732805038	0.44262664845470	n
2.06079980354008	0.61078546738212	-1.30448136798935	h
-2.06079980354008	-0.61078546738212	-1.30448136798935	h
2.08747379308132	-1.63000779480150	0.86185471953465	h
-2.08747379308132	1.63000779480150	0.86185471953465	h

N_4

```
  0.97352637877574      0.97353427649995      0.97350854749399      n
 -0.97347107666161      0.97345970934768     -0.97348952076396      n
 -0.97352288698680     -0.97351512802877      0.97348592757745      n
  0.97346758487266     -0.97347885781885     -0.97350495430747      n
```

Na_2

```
  2.96175863265435      0.00000000000000      0.00000000000000      na
 -2.96175863265435      0.00000000000000      0.00000000000000      na
```

Na_2O

```
  0.00000000000000      0.00000000000000     -0.00125987003817      o
  3.76616708679694      0.00000000000000      0.00062993501909      na
 -3.76616708679694      0.00000000000000      0.00062993501909      na
```

Na_2S

```
  0.00000000000000      0.00000000000000      0.00000000000000      s
  0.00000000000000      0.00000000000000     -4.54664766104049      na
  0.00000000000000      0.00000000000000      4.54664766104049      na
```

Na_3N

```
  0.00000000000000      0.00000000000000      0.98846813029527      n
 -1.94602685234149      3.37061738114880     -0.32948937676509      na
 -1.94602685234149     -3.37061738114880     -0.32948937676509      na
  3.89205370468299      0.00000000000000     -0.32948937676509      na
```

Na_3P

```
  0.02166950952763     -0.00927750719924      1.85753834100637      p
  1.53863108521887     -3.99579517958087     -0.62708109943298      na
  2.65769485647032      3.35118326979984     -0.62224016723425      na
 -4.21799545121683      0.65388941698028     -0.60821707433915      na
```

NaCl

```
  0.00000000000000      0.00000000000000     -2.23125548600731      na
  0.00000000000000      0.00000000000000      2.23125548600731      cl
```

NaF

```
  0.00000000000000      0.00000000000000     -1.81647944104883      na
  0.00000000000000      0.00000000000000      1.81647944104883      f
```

NaH

```
  0.00000000000000      0.00000000000000     -1.79420308214526      na
  0.00000000000000      0.00000000000000      1.79420308214526      h
```

NbO_2F

```
 -0.07885652263078     -0.85949293909304      0.00000000000000      nb
 -1.65929655990476      0.34938939767406      2.62884799697737      o
 -1.65929655990476      0.34938939767406     -2.62884799697737      o
  3.39744964244030      0.16071414374492      0.00000000000000      f
```

Ne_2

```
  0.00000000000000      0.00000000000000     -2.59159992926640      ne
  0.00000000000000      0.00000000000000      2.59159992926640      ne
```

NF_3

-0.00023917863373	0.86723125260972	0.00000000000000	n
2.36152560364088	-0.29019299685791	0.00000000000000	f
-1.18064321250358	-0.28851912787590	2.04401593693485	f
-1.18064321250358	-0.28851912787590	-2.04401593693485	f

NH_3

-0.00002996273382	0.60419573896846	0.00000000000000	n
1.77459787410351	-0.20146478753319	0.00000000000000	h
-0.88728395568485	-0.20136547571764	1.53702086353764	h
-0.88728395568485	-0.20136547571764	-1.53702086353764	h

NH_4F

0.00035295142012	0.99586270905472	0.00000000000000	n
1.79756586681634	1.73917600761303	0.00000000000000	h
-0.89974980156668	1.73568143900128	1.55739131188531	h
-0.89974980156668	1.73568143900128	-1.55739131188531	h
0.00153471995548	-2.18853841134706	0.00000000000000	h
0.00004606494142	-4.01786318332326	0.00000000000000	f

$Ni(CO)_4$

0.00000000000000	0.00000000000000	0.00000000000000	ni
1.98326378231725	-1.98326378231725	1.98326378231725	c
-1.98326378231725	1.98326378231725	1.98326378231725	c
-1.98326378231725	-1.98326378231725	-1.98326378231725	c
1.98326378231725	1.98326378231725	-1.98326378231725	c
3.24273654096679	-3.24273654096679	3.24273654096679	o
-3.24273654096679	3.24273654096679	3.24273654096679	o
-3.24273654096679	-3.24273654096679	-3.24273654096679	o
3.24273654096679	3.24273654096679	-3.24273654096679	o

OF_2

0.00000000000000	0.00000000000000	1.08966458588793	o
-2.12636045821744	0.00000000000000	-0.54483229294396	f
2.12636045821744	0.00000000000000	-0.54483229294396	f

$Os(CO)_5$

0.00000000000000	0.00000000000000	0.00000000000000	os
1.86245714222963	-3.22587039726125	0.00000000000000	c
1.86245714222963	3.22587039726125	0.00000000000000	c
-3.72491428445925	0.00000000000000	0.00000000000000	c
0.00000000000000	0.00000000000000	3.74847701997556	c
0.00000000000000	0.00000000000000	-3.74847701997556	c
2.95959230898802	-5.12616424885734	0.00000000000000	o
2.95959230898802	5.12616424885734	0.00000000000000	o
-5.91918461797604	0.00000000000000	0.00000000000000	o
0.00000000000000	0.00000000000000	5.93170395303675	o
0.00000000000000	0.00000000000000	-5.93170395303675	o

OsO_3

0.00000000000000	0.00000000000000	0.00000000000000	os
1.63177166219432	-2.82631142527168	0.00000000000000	o
1.63177166219432	2.82631142527168	0.00000000000000	o
-3.26354332438864	0.00000000000000	0.00000000000000	o

OsO_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      os
  1.90033009057400     -1.90033009057400      1.90033009057400      o
 -1.90033009057400      1.90033009057400      1.90033009057400      o
 -1.90033009057400     -1.90033009057400     -1.90033009057400      o
  1.90033009057400      1.90033009057400     -1.90033009057400      o
```

P_2

```
  0.00000000000000      0.00000000000000      1.81038834147637      p
  0.00000000000000      0.00000000000000     -1.81038834147637      p
```

PbH_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      pb
  1.91301550123300     -1.91301550123300      1.91301550123300      h
 -1.91301550123300      1.91301550123300      1.91301550123300      h
 -1.91301550123300     -1.91301550123300     -1.91301550123300      h
  1.91301550123300      1.91301550123300     -1.91301550123300      h
```

PbO_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      pb
  0.00000000000000      0.00000000000000      3.61357863592328      o
  0.00000000000000      0.00000000000000     -3.61357863592328      o
```

PbO

```
  0.00000000000000      0.00000000000000     -1.80754257937630      pb
  0.00000000000000      0.00000000000000      1.80754257937630      o
```

$PdBr_2$

```
  0.00000000000000      0.00000000000000      1.94736786722181      pd
  3.32052092225479      0.00000000000000     -0.97368393361090      br
 -3.32052092225479      0.00000000000000     -0.97368393361090      br
```

$Pd(CO)_4$

```
  0.00000919143467      0.00000531380106     -0.00001191622877      pd
  2.18351277656177      2.18350949811326      2.18351805760958      c
 -2.18350195361372     -2.18350090015659      2.18350128273601      c
  2.18351494366302     -2.18352263605300     -2.18351671330313      c
 -2.18351964856344      2.18351087841231     -2.18351593700892      c
  3.44064404148229      3.44064088770018      3.44067413451479      o
 -3.44064406985283     -3.44062025793711      3.44067735832652      o
  3.44066163241694     -3.44068081079362     -3.44066336280415      o
 -3.44067691352870      3.44065802691347     -3.44066290384197      o
```

PF_2

```
  0.00190593228732      0.00000637856307     -1.13522248396255      p
  2.65740159746508      0.00000628935462      0.38170793256163      f
 -1.32964926884328      2.29968766474854      0.37675740109626      f
 -1.32965826090911     -2.29970033266624      0.37675715030465      f
```

PF_5

```
  0.00093568540199      0.00000556340549      0.00000000000000      p
  0.00115403835462     -3.04805754510344      0.00000000000000      f
  0.00115453827044      3.04805857150255      0.00000000000000      f
  3.00853565827311     -0.00000245516935      0.00000000000000      f
 -1.50588996015008     -0.00000206731762      2.60331280562780      f
 -1.50588996015008     -0.00000206731762     -2.60331280562780      f
```

PH_3

```
  0.00021868262881      0.00000408524970     -1.13254033248507      p
  2.26639108333582      0.00000455950564      0.37803102689817      h
 -1.13330963847505      1.96296552283309      0.37726390137846      h
 -1.13330012748958     -1.96297416758843      0.37724540420844      h
```

Li_3P

```
 -0.00040508715227      1.96231380420593      0.00000000000000      p
  3.47020495828402     -0.65597305055359      0.00000000000000      li
 -1.73489993556587     -0.65317037682617      3.00666083679482      li
 -1.73489993556587     -0.65317037682617     -3.00666083679482      li
```

$PoBr_2$

```
  0.00000000000000      0.00000000000000     -2.05077811234213      po
 -3.91000444459516      0.00000000000000      1.02538905617107      br
  3.91000444459516      0.00000000000000      1.02538905617107      br
```

$PoCl_4$

```
  0.00000000000000      0.00000000000000     -0.04743067470634      po
  0.00000000000000      0.00000000000000      4.74833316645761      cl
  2.28262919289879      3.95362973694065     -1.56696749725042      cl
  2.28262919289879     -3.95362973694065     -1.56696749725042      cl
 -4.56525838579759      0.00000000000000     -1.56696749725042      cl
```

PoF_2

```
  0.00000000000000      0.00000000000000      1.69785932644653      po
  2.90641662530823      0.00000000000000     -0.84892966322327      f
 -2.90641662530823      0.00000000000000     -0.84892966322327      f
```

PoF_6

```
  0.00000000000000      0.00000000000000      0.00000000000000      po
  0.00000000000000      3.82106639815121      0.00000000000000      f
  0.00000000000000      0.00000000000000      3.82106639815121      f
  3.82106639815121      0.00000000000000      0.00000000000000      f
  0.00000000000000      0.00000000000000     -3.82106639815121      f
 -3.82106639815121      0.00000000000000      0.00000000000000      f
  0.00000000000000     -3.82106639815121      0.00000000000000      f
```

PoO_2

```
  0.00000000000000      0.00000000000000     -1.45547913397531      po
 -2.99786658909094      0.00000000000000      0.72773956698766      o
  2.99786658909094      0.00000000000000      0.72773956698766      o
```

$Pt(CO)_4$

```
  0.00000000000000      0.00000000000000      0.00000000000000      pt
  2.17219503977633     -2.17219503977633      2.17219503977633      c
 -2.17219503977633      2.17219503977633      2.17219503977633      c
 -2.17219503977633     -2.17219503977633     -2.17219503977633      c
  2.17219503977633      2.17219503977633     -2.17219503977633      c
  3.43196912076035     -3.43196912076035      3.43196912076035      o
 -3.43196912076035      3.43196912076035      3.43196912076035      o
 -3.43196912076035     -3.43196912076035     -3.43196912076035      o
  3.43196912076035      3.43196912076035     -3.43196912076035      o
```

PtO_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      pt
  0.00000000000000      0.00000000000000     -3.28869598692728      o
  0.00000000000000      0.00000000000000      3.28869598692728      o
```

Rb_2

```
  0.00000000000000      0.00000000000000      4.02929309031907      rb
  0.00000000000000      0.00000000000000     -4.02929309031907      rb
```

RbF

```
  0.00000000000000      0.00000000000000     -2.29684487633273      f
  0.00000000000000      0.00000000000000      2.29684487633273      rb
```

RbH

```
  0.00000000000000      0.00000000000000     -2.33735012066011      rb
  0.00000000000000      0.00000000000000      2.33735012066011      h
```

Re_2O_7

```
  0.00000000000000      0.00000000000000      0.00000000000000      o
  0.00000000000000      0.00000000000000      3.59816208139028      re
  0.00000000000000      0.00000000000000     -3.59816208139028      re
  2.65284876142376     -1.53162294652736      4.76018070105388      o
  2.65284876142376      1.53162294652736     -4.76018070105388      o
  0.00000000000000      3.06324589305468      4.76018070105388      o
 -2.65284876142376      1.53162294652736     -4.76018070105388      o
 -2.65284876142376     -1.53162294652736      4.76018070105388      o
  0.00000000000000     -3.06324589305468     -4.76018070105388      o
```

Rn_2

```
  0.00000000000000      0.00000000000000     -2.55668948172277      rn
  0.00000000000000      0.00000000000000      2.55668948172277      rn
```

RnF_2

```
  0.00000000000000     -2.13005357562107      0.00000000000000      rn
 -2.19568861249798      1.06502678781053      0.00000000000000      f
  2.19568861249798      1.06502678781053      0.00000000000000      f
```

$Ru(CO)_5$

```
  0.00000000000000      0.00000000000000      0.00000000000000      ru
  1.84480011535838     -3.19528752960964      0.00000000000000      c
  1.84480011535838      3.19528752960964      0.00000000000000      c
 -3.68960023071676      0.00000000000000      0.00000000000000      c
  0.00000000000000      0.00000000000000      3.69125554048716      c
  0.00000000000000      0.00000000000000     -3.69125554048716      c
  2.94039490193387     -5.09291336446596      0.00000000000000      o
  2.94039490193387      5.09291336446596      0.00000000000000      o
 -5.88078980386773      0.00000000000000      0.00000000000000      o
  0.00000000000000      0.00000000000000      5.87379294085885      o
  0.00000000000000      0.00000000000000     -5.87379294085885      o
```

RuO_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      ru
  0.00000000000000      0.00000000000000      3.22936844775946      o
  0.00000000000000      0.00000000000000     -3.22936844775946      o
```

RuO_4

```
 -0.00003901512132     -0.00004974867915      0.00003175074579      ru
  1.87142850130396      1.87147977103538      1.87148905199029      o
 -1.87142232278019     -1.87137312944410      1.87142093412647      o
  1.87151789303364     -1.87153124203117     -1.87151937514838      o
 -1.87148505643610      1.87147434911906     -1.87142236171416      o
```

S_5

```
 -1.01219286085597      0.91031071217532      2.78939529359939      s
  2.56254320877922     -0.26701145071347      2.27262712733185      s
  2.56256180032893     -0.26700825963793     -2.27262274065567      s
 -1.01216802810249      0.91029852260584     -2.78940508703009      s
 -3.10074412014967     -1.28658952442978      0.00000540675450      s
```

SbF_2

```
  0.00000000000000      0.00000000000000      1.41635010067847      sb
 -1.57661128992144      2.73077085793065     -0.47211670022616      f
 -1.57661128992144     -2.73077085793065     -0.47211670022616      f
  3.15322257984289      0.00000000000000     -0.47211670022616      f
```

SbH_3

```
  0.00000000000000      0.00000000000000      1.40288124678412      sb
  1.34916589534128     -2.33682387857025     -0.46762708226138      h
  1.34916589534128      2.33682387857025     -0.46762708226138      h
 -2.69833179068256      0.00000000000000     -0.46762708226138      h
```

$ScCl_3$

```
  0.00000000000000      0.00000000000000      0.00000000000000      sc
  2.15416668810895     -3.73112615177708      0.00000000000000      cl
  2.15416668810895      3.73112615177708      0.00000000000000      cl
 -4.30833337621790      0.00000000000000      0.00000000000000      cl
```

ScF_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      sc
  1.73202055035891     -2.99994759297505      0.00000000000000      f
  1.73202055035891      2.99994759297505      0.00000000000000      f
 -3.46404110071783      0.00000000000000      0.00000000000000      f
```

ScH_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      sc
  1.71347214324408     -2.96782080945268      0.00000000000000      h
  1.71347214324408      2.96782080945268      0.00000000000000      h
 -3.42694428648816      0.00000000000000      0.00000000000000      h
```

Se_8

```
  4.73473332107232     -1.96119075580796      1.08203483157154      se
  1.96119075580796      4.73473332107232      1.08203483157154      se
 -4.73473332107232      1.96119075580796      1.08203483157154      se
 -1.96119075580796     -4.73473332107232      1.08203483157154      se
  4.73473332107232      1.96119075580796     -1.08203483157154      se
 -1.96119075580796      4.73473332107232     -1.08203483157154      se
 -4.73473332107232     -1.96119075580796     -1.08203483157154      se
  1.96119075580796     -4.73473332107232     -1.08203483157154      se
```

SeH_2

0.00000000000000	0.00000000000000	1.31443756714499	se
-1.99442696033084	0.00000000000000	-0.65721878357249	h
1.99442696033084	0.00000000000000	-0.65721878357249	h

SeO_2

0.00000000000000	0.00000000000000	1.10091950638887	se
-2.61260008861725	0.00000000000000	-0.55045975319444	o
2.61260008861725	0.00000000000000	-0.55045975319444	o

SF_2

0.00000000000000	0.00000000000000	1.32266337773884	s
2.37880811467657	0.00000000000000	-0.66133188418768	f
-2.37880811467657	0.00000000000000	-0.66133188418768	f

SF_4

-0.00000226380055	-0.00002431422764	0.84926009844488	s
-3.18886562268367	-0.00001733471558	0.66640784370306	f
3.18886006659826	-0.00001733422028	0.66642737569287	f
0.00000390405808	2.35445661105741	-1.09097973125881	f
0.00000391582787	-2.35439762789392	-1.09111558658199	f

SF_6

0.00000000000000	0.00000000000000	0.00000118515990	s
-2.15172851914079	-2.15172851914079	-0.00000033099473	f
0.00000000000000	0.00000000000000	3.04300291311907	f
-2.15172851914079	2.15172851914079	-0.00000033099473	f
0.00000000000000	0.00000000000000	-3.04300276329175	f
2.15172851914079	-2.15172851914079	-0.00000033099473	f
2.15172851914079	2.15172851914079	-0.00000033099473	f

$SiCl_4$

0.00000000000000	0.00000000000000	0.00000000000000	si
2.24180189786400	-2.24180189786400	2.24180189786400	cl
-2.24180189786400	2.24180189786400	2.24180189786400	cl
-2.24180189786400	-2.24180189786400	-2.24180189786400	cl
2.24180189786400	2.24180189786400	-2.24180189786400	cl

SiF_4

0.00000000000000	0.00000000000000	0.00000000000000	si
1.74748733068482	-1.74748733068482	1.74748733068482	f
-1.74748733068482	1.74748733068482	1.74748733068482	f
-1.74748733068482	-1.74748733068482	-1.74748733068482	f
1.74748733068482	1.74748733068482	-1.74748733068482	f

SiH_4

0.00000000000000	0.00000000000000	0.00000000000000	si
1.63806238513397	-1.63806238513397	1.63806238513397	h
-1.63806238513397	1.63806238513397	1.63806238513397	h
-1.63806238513397	-1.63806238513397	-1.63806238513397	h
1.63806238513397	1.63806238513397	-1.63806238513397	h

SiO_2

0.00000000000000	0.00000000000000	0.00000000000000	si
0.00000000000000	0.00000000000000	-2.90863957585795	o
0.00000000000000	0.00000000000000	2.90863957585795	o

SiS_2

0.00000000000000	0.00000000000000	0.00000000000000	si
0.00000000000000	0.00000000000000	-3.68153174204543	s
0.00000000000000	0.00000000000000	3.68153174204543	s

SnH_4

0.00000000000000	0.00000000000000	0.00000000000000	sn
1.89044177023958	-1.89044177023958	1.89044177023958	h
-1.89044177023958	1.89044177023958	1.89044177023958	h
-1.89044177023958	-1.89044177023958	-1.89044177023958	h
1.89044177023958	1.89044177023958	-1.89044177023958	h

SnO_2

```
  0.00000000000000      0.00000000000000      0.00163548812459      sn
 -3.51460840178293      0.00000000000000     -0.00081774406230      o
  3.51460840178293      0.00000000000000     -0.00081774406230      o
```

SnO

```
  0.00000000000000      0.00000000000000     -1.76719363698803      sn
  0.00000000000000      0.00000000000000      1.76719363698803      o
```

Sr_4

```
  2.21018294136508     -2.21018294136508      2.21018294136508      sr
 -2.21018294136508      2.21018294136508      2.21018294136508      sr
 -2.21018294136508     -2.21018294136508     -2.21018294136508      sr
  2.21018294136508      2.21018294136508     -2.21018294136508      sr
```

SrF_2

```
  0.00000000000000      0.00000000000000      1.21686253050211      sr
  3.54167198526231      0.00000000000000     -0.60843126525105      f
 -3.54167198526231      0.00000000000000     -0.60843126525105      f
```

SrH_2

```
  0.00000000000000      0.00000000000000      1.36780798604125      sr
 -3.52443250853761      0.00000000000000     -0.68390399302062      h
  3.52443250853761      0.00000000000000     -0.68390399302062      h
```

SrO

```
  0.00000000000000      0.00000000000000     -1.83598401421036      sr
  0.00000000000000      0.00000000000000      1.83598401421036      o
```

SrS

```
  0.00000000000000      0.00000000000000     -2.31673677279564      sr
  0.00000000000000      0.00000000000000      2.31673677279564      s
```

TaF_4

```
  0.00000000000000      0.00000000000000     -0.00088004990885      ta
 -1.76481713541870      3.05675294461335      0.00029334996962      f
 -1.76481713541870     -3.05675294461335      0.00029334996962      f
  3.52963427083740      0.00000000000000      0.00029334996962      f
```

TaO_2F

```
  0.00000000000000      0.00000000000000      0.03006542312973      ta
  0.00000000000000      0.00000000000000      3.72739793762169      f
  2.74274130577697      0.00000000000000     -1.87873168037571      o
 -2.74274130577697      0.00000000000000     -1.87873168037571      o
```

TcO_7

```
  0.00000000000000      0.00000000000000      0.00000000000000      o
  0.00000000000000      0.00000000000000      3.55098914866315      tc
  0.00000000000000      0.00000000000000     -3.55098914866315      tc
  2.62571861860354     -1.51595935126696      4.65860875354015      o
  2.62571861860354      1.51595935126696     -4.65860875354015      o
  0.00000000000000      3.03191870253393      4.65860875354015      o
 -2.62571861860354      1.51595935126696     -4.65860875354015      o
 -2.62571861860354     -1.51595935126696      4.65860875354015      o
  0.00000000000000     -3.03191870253393     -4.65860875354015      o
```

TcO_3F

```
  0.00000000000000      0.00000000000000     -0.03575380241616      tc
  0.00000000000000      0.00000000000000      3.47832150786421      f
  1.51189127548743     -2.61867250466434     -1.14752256848268      o
  1.51189127548743      2.61867250466434     -1.14752256848268      o
 -3.02378255097485      0.00000000000000     -1.14752256848268      o
```

TeH_2

```
  0.00000000000000      0.00000000000000      1.49820193039170      te
 -2.24906865611118      0.00000000000000     -0.74910096519585      h
  2.24906865611118      0.00000000000000     -0.74910096519585      h
```

TeO_2

```
  0.00000000000000      0.00000000000000      1.29984292231352      te
 -2.88498675314837      0.00000000000000     -0.64992146115676      o
  2.88498675314837      0.00000000000000     -0.64992146115676      o
```

$TiCl_4$

```
  0.00000000000000      0.00000000000000      0.00000000000000      ti
  2.38225918250055     -2.38225918250055      2.38225918250055      cl
 -2.38225918250055      2.38225918250055      2.38225918250055      cl
 -2.38225918250055     -2.38225918250055     -2.38225918250055      cl
  2.38225918250055      2.38225918250055     -2.38225918250055      cl
```

$Ti(CO)_4$

```
  0.00000000000000      0.00000000000000      0.00000000000000      ti
  2.25209609785139     -2.25209609785139      2.25209609785139      c
 -2.25209609785139      2.25209609785139      2.25209609785139      c
 -2.25209609785139     -2.25209609785139     -2.25209609785139      c
  2.25209609785139      2.25209609785139     -2.25209609785139      c
  3.52294080235074     -3.52294080235074      3.52294080235074      o
 -3.52294080235074      3.52294080235074      3.52294080235074      o
 -3.52294080235074     -3.52294080235074     -3.52294080235074      o
  3.52294080235074      3.52294080235074     -3.52294080235074      o
```

TiF_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      ti
  1.91049002205680     -1.91049002205680      1.91049002205680      f
 -1.91049002205680      1.91049002205680      1.91049002205680      f
 -1.91049002205680     -1.91049002205680     -1.91049002205680      f
  1.91049002205680      1.91049002205680     -1.91049002205680      f
```

TiH_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      ti
  1.85401673992524     -1.85401673992524      1.85401673992524      h
 -1.85401673992524      1.85401673992524      1.85401673992524      h
 -1.85401673992524     -1.85401673992524     -1.85401673992524      h
  1.85401673992524      1.85401673992524     -1.85401673992524      h
```

TiO_2

```
  0.00000000000000      0.00000000000000      1.20428895304113      ti
 -2.52745691819368      0.00000000000000     -0.60214447652056      o
  2.52745691819368      0.00000000000000     -0.60214447652056      o
```

TiS_2

```
  0.00000000000000      0.00000000000000      1.47408703528939      ti
 -3.26474084717958      0.00000000000000     -0.73704351764470      s
  3.26474084717958      0.00000000000000     -0.73704351764470      s
```

$TlCl_3$

```
  0.00000000000000      0.00000000000000     -0.01443837177572      tl
 -2.26117878730255      3.91647654460500      0.00481279059057      cl
 -2.26117878730255     -3.91647654460500      0.00481279059057      cl
  4.52235757460510      0.00000000000000      0.00481279059057      cl
```

TlCl

```
  0.00000000000000      0.00000000000000     -2.38342001986092      tl
  0.00000000000000      0.00000000000000      2.38342001986092      cl
```

TlH_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      tl
 -1.64536913789863      2.84986294404622      0.00000000000000      h
 -1.64536913789863     -2.84986294404622      0.00000000000000      h
  3.29073827579725      0.00000000000000      0.00000000000000      h
```

TlH

```
  0.00000000000000      0.00000000000000     -1.81347675018980      tl
  0.00000000000000      0.00000000000000      1.81347675018980      h
```

VH_5

```
  0.00000000000000      0.00000000000000     -0.57064280187526      v
  0.00000000000000      0.00000000000000     -3.72869229559981      h
  1.83996677045142     -1.83997133446016      1.07483377436877      h
  1.83996677045142      1.83997133446016      1.07483377436877      h
 -1.83996677045142      1.83997133446016      1.07483377436877      h
 -1.83996677045142     -1.83997133446016      1.07483377436877      h
```

$W(CO)_6$

```
  0.00000000000000      0.00000000000000      0.00000000000000      w
  0.00000000000000      3.93720141856123      0.00000000000000      c
  0.00000000000000      0.00000000000000      3.93720141856123      c
  3.93720141856123      0.00000000000000      0.00000000000000      c
  0.00000000000000      0.00000000000000     -3.93720141856123      c
 -3.93720141856123      0.00000000000000      0.00000000000000      c
  0.00000000000000     -3.93720141856123      0.00000000000000      c
  0.00000000000000      6.12568593744740      0.00000000000000      o
  0.00000000000000      0.00000000000000      6.12568593744740      o
  6.12568593744740      0.00000000000000      0.00000000000000      o
  0.00000000000000      0.00000000000000     -6.12568593744740      o
 -6.12568593744740      0.00000000000000      0.00000000000000      o
  0.00000000000000     -6.12568593744740      0.00000000000000      o
```

WO_3

```
  0.00000000000000      0.00000000000000      0.00000000000000      w
  1.67015014718729     -2.89278491119702      0.00000000000000      o
  1.67015014718729      2.89278491119702      0.00000000000000      o
 -3.34030029437458      0.00000000000000      0.00000000000000      o
```

XeF_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      xe
  0.00000000000000      0.00000000000000      3.90757878328295      f
  0.00000000000000      0.00000000000000     -3.90757878328295      f
```

XeF_4

```
  0.00000000000000      0.00000000000000      0.00000000000000      xe
  2.72236103703447     -2.72236103703447      0.00000000000000      f
  2.72236103703447      2.72236103703447      0.00000000000000      f
 -2.72236103703447      2.72236103703447      0.00000000000000      f
 -2.72236103703447     -2.72236103703447      0.00000000000000      f
```

$XeOF_4$

```
  0.00000000000000      0.00000000000000     -0.39099828949089      xe
  0.00000000000000      0.00000000000000      3.04665434896357      o
  2.70138310369918     -2.70138310369918     -0.66391401486817      f
  2.70138310369918      2.70138310369918     -0.66391401486817      f
 -2.70138310369918      2.70138310369918     -0.66391401486817      f
 -2.70138310369918     -2.70138310369918     -0.66391401486817      f
```

YF_3

```
  0.00000000000000      0.00000000000000      0.00977112603694      y
 -1.89922978387516      3.28956248091983     -0.00325704201177      f
 -1.89922978387516     -3.28956248091983     -0.00325704201177      f
  3.79845956775031      0.00000000000000     -0.00325704201177      f
```

YF

```
  0.00000000000000      0.00000000000000     -1.84234806551158      y
  0.00000000000000      0.00000000000000      1.84234806551158      f
```

Zn_2

```
  0.00000000000000      0.00000000000000     -3.05568801489619      zn
  0.00000000000000      0.00000000000000      3.05568801489619      zn
```

$ZnCl_2$

```
  0.00000000000000      0.00000000000000      0.00000000000000      zn
  0.00000000000000      0.00000000000000      3.97259040076298      cl
  0.00000000000000      0.00000000000000     -3.97259040076298      cl
```

ZnF_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      zn
  0.00000000000000      0.00000000000000      3.28287621534218      f
  0.00000000000000      0.00000000000000     -3.28287621534218      f
```

ZnH_2

```
  0.00000000000000      0.00000000000000      0.00000000000000      zn
  0.00000000000000      0.00000000000000     -2.92711569055511      h
  0.00000000000000      0.00000000000000      2.92711569055511      h
```

$Zn(CH_3)_2$

```
 -3.68550740141615      0.00000000000000      0.00000000000000      c
  3.68550740141615      0.00000000000000      0.00000000000000      c
 -4.45127468148499      1.69783313045575     -0.98024441490769      h
 -4.45127468148499      0.00000000000000      1.96048882981538      h
 -4.45127468148499     -1.69783313045575     -0.98024441490769      h
  4.45127468148499     -1.69783313045575     -0.98024441490769      h
  4.45127468148499      0.00000000000000      1.96048882981538      h
  4.45127468148499      1.69783313045575     -0.98024441490769      h
  0.00000000000000      0.00000000000000      0.00000000000000      zn
```

ZrO_2

```
  0.00000000000000      0.00000000000000      1.36096020616404      zr
 -2.71171774062042      0.00000000000000     -0.68048010308202      o
  2.71171774062042      0.00000000000000     -0.68048010308202      o
```

ZrO

```
  0.00000000000000      0.00000000000000     -1.66498802952802      zr
  0.00000000000000      0.00000000000000      1.66498802952802      o
```

3 NMR shielding constants of the studied molecules

The uncontracted ANO-RCC bases[12–15] were employed with the PBE0[16,17] functional and the PBE[16] functional. Calculations with other basis sets were only performed with the PBE functional. For comparison, we choose the Karlsruhe x2c-TZVPall, x2c-TZVPall-2c, x2c-TZVPPall bases[1] (here abbreviated as TZVPall etc.), the contracted Sapporo triple-ζ[18,19] (Sapporo-TZP-2012 and Sappro-DKH3-TZP-2012, here abbreviated as Sapporo-TZP) and Dyall's uncontracted triple-ζ valence[20–26] (Dyall-VTZ) set. Decontraction was done as suggested by Dyall and Dunning's uncontracted cc-pVTZ bases[27] were used for the lighter elements (1s to 3p, and 3d). A large even-tempered (ET) reference basis set[1] is used to assess the quality. Further the corresponding double-ζ basis sets were studied. The threshold for the SCF calculation was set to $10^{-8}\,E_\mathrm{h}$ and fine grids (grid 4a) were used for numerical integration of the exchange correlation potential in DFT. All calculations were performed with TURBOMOLE[6–8] and its X2C implementation[4,5,28] with the finite nucleus model. For details see the main text. The results are sorted according to the group of the element of interest.

3.1 Triple-zeta basis sets

3.1.1 Group 1s

Table 3 NMR isotropic shielding constants of various molecules containing 1s elements. Organic H-NMR chemical shifts span a range of roughly 10 ppm.[29]

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
AlH_3	25.5	25.8	25.5	25.5	25.5	25.5	25.5	25.6	25.5
AsH_3	28.6	28.6	28.6	28.6	28.6	28.7	28.6	28.7	28.6
B_2H_6	31.4	31.6	31.4	31.4	31.3	31.2	31.1	31.2	31.4
B_2H_6	26.3	26.6	26.3	26.3	26.4	26.6	26.5	26.6	26.3
$B_3N_3H_6$	26.1	26.3	26.1	26.2	26.3	26.6	26.5	26.6	26.2
$B_3N_3H_6$	25.1	25.4	25.1	25.1	25.1	25.9	25.5	25.9	25.2
B_4H_4	19.9	19.9	19.9	20.0	19.9	20.0	19.9	20.0	19.9
BaH_2	23.3	23.5	23.2	23.3	23.4	23.0	23.2	23.0	23.0
Be_2H_4	25.8	26.3	25.9	25.9	25.6	25.7	25.7	25.7	25.7
Be_2H_4	26.0	26.6	26.4	26.4	26.4	25.5	25.6	25.5	25.5
BeC_2H_6	31.7	31.7	31.6	31.7	31.6	31.9	31.6	31.9	31.7
$BeF_2O_2H_4$	28.2	28.0	28.2	28.5	28.5	29.2	28.7	29.2	28.6
BeH_2	27.4	28.0	28.0	27.9	27.7	26.7	26.8	26.7	26.6
BH_3	22.7	23.0	22.7	22.7	22.7	22.8	22.7	22.8	22.7
BH_3CO	29.5	29.6	29.5	29.5	29.5	29.6	29.5	29.6	29.5
BH_3NH_3	28.8	29.0	28.8	28.9	28.9	29.1	29.0	29.1	28.9
BH_3NH_3	28.1	28.3	28.1	28.3	28.2	28.7	28.3	28.7	28.4
BiH_3	27.0	27.0	27.0	27.0	27.0	27.1	27.0	27.1	27.0
C_2H_2	29.7	29.6	29.7	29.8	29.3	29.0	28.9	29.0	29.6
C_2H_3N	30.9	30.9	30.9	31.2	31.0	31.6	31.2	31.6	31.1
C_2H_3N	23.7	23.6	23.7	23.8	23.4	23.3	23.1	23.3	23.6
C_2H_4	25.2	25.3	25.2	25.3	25.5	26.0	25.7	26.0	25.3
C_2H_6	30.0	30.1	30.0	30.1	30.0	30.2	30.0	30.2	30.1
C_4H_4	28.0	27.8	28.0	28.1	28.0	28.3	28.1	28.3	28.1
C_6H_6	23.4	23.4	23.4	23.6	23.6	24.2	23.9	24.2	23.6
CaH_2	26.0	26.0	25.9	25.8	25.8	25.7	25.8	25.7	25.7
$Cd(CH_3)_2$	31.1	31.3	31.1	31.2	31.1	31.3	31.1	31.3	31.2
CH_2O	20.5	20.9	20.5	20.7	20.9	21.4	21.2	21.4	20.7
CH_2O_2	25.9	26.1	25.9	25.9	25.9	26.1	26.0	26.1	25.9
CH_3N	20.3	20.4	20.3	20.3	20.5	21.3	21.0	21.3	20.4
CH_3N	22.5	22.8	22.5	22.7	22.9	23.4	23.2	23.4	22.7
CH_3N	23.0	23.1	23.0	23.2	23.3	23.8	23.6	23.8	23.2
CH_4	30.8	30.8	30.8	30.9	30.8	31.1	30.9	31.1	23.2
CsH	24.2	24.4	24.1	24.2	24.0	24.0	24.1	24.0	30.9
CuH	33.3	31.6	33.3	33.8	35.2	33.6	33.4	33.5	33.4
Ferrocene	27.0	27.2	27.0	27.2	27.1	27.6	27.4	27.6	27.2
GaH_3	24.2	24.6	24.2	24.2	24.2	24.4	24.3	24.4	24.3
GeH_4	27.1	27.2	27.1	27.2	27.1	27.2	27.2	27.2	27.1
H_2	26.2	26.2	26.2	26.3	26.2	26.3	26.2	26.3	26.2
H_2CO_3	25.8	25.6	25.8	26.2	26.1	26.9	26.4	26.9	26.1
H_2O	30.8	30.5	30.8	31.1	31.0	31.6	31.2	31.6	31.0
H_2O_2	24.3	24.5	24.3	24.7	24.5	25.0	24.6	25.0	24.6
H_2SO_4	26.1	26.0	26.0	26.6	26.3	26.8	26.4	26.7	26.4
H_3PO_4	27.5	27.4	27.5	27.9	27.7	28.4	27.9	28.4	27.8
HBr	31.1	30.7	31.1	31.1	31.0	31.2	31.0	31.2	31.0
$CHBr_3$	22.4	23.0	22.4	22.5	22.2	22.3	22.0	22.3	22.6
HCl	30.7	30.4	30.8	30.9	30.7	31.0	30.7	30.8	30.7
HCN	28.3	28.3	28.3	28.4	27.8	27.4	27.3	27.4	28.2
HCP	28.8	28.9	28.8	28.8	28.2	27.8	27.7	27.8	28.7
He_2	59.9	59.8	59.7	59.8	59.8	59.8	59.8	59.8	59.8
HF	29.3	28.7	29.3	29.6	29.4	29.8	29.4	29.8	29.5
$Hg(CH_3)_2$	30.7	30.9	30.7	30.8	30.8	31.1	30.8	31.1	30.8
HI	27.1	27.1	27.0	27.1	26.5	26.4	26.1	26.4	27.0
HNC	1.0	1.0	1.0	0.4	1.9	2.9	2.6	2.9	1.0
HNO	16.3	16.6	16.3	16.6	16.5	17.3	16.9	17.3	16.6
HNO_2	21.2	20.9	21.2	21.7	21.5	22.1	21.6	22.1	21.5
HNO_3	30.3	30.1	30.3	30.4	30.3	30.5	30.3	30.9	30.3
H_2S	27.5	27.6	27.5	27.7	27.5	27.8	27.6	27.5	27.6
H_2S_2	31.2	30.8	31.2	31.2	31.0	31.2	31.1	31.2	31.1

InH	21.8	22.1	21.8	21.7	21.6	21.5	21.5	21.5	21.5
InH_3	21.8	24.7	24.3	24.3	24.3	24.4	24.3	24.4	24.4
KH	24.9	25.2	24.9	25.0	24.9	24.8	24.8	24.8	24.8
LaH_3	21.9	22.3	21.9	21.8	21.8	21.8	21.9	21.8	21.8
$Li_4C_4H_{12}$	32.6	32.7	32.6	32.7	32.6	33.0	32.7	33.0	32.7
Li_4H_4	27.7	27.8	27.7	27.7	27.7	27.9	27.7	27.9	27.8
$LiBH_4$	30.2	30.3	30.2	30.3	30.2	30.3	30.2	30.3	30.2
$LiBH_4$	31.3	31.4	31.4	31.4	31.3	31.3	31.3	31.3	31.4
LiH	26.1	26.3	26.2	26.1	26.2	26.0	26.1	26.0	26.0
MgH_2	26.5	26.7	26.5	26.5	26.6	26.3	26.3	26.2	26.3
H_2N_2	14.3	14.7	14.3	14.4	14.8	15.7	15.3	15.7	14.6
N_2H_4	28.0	28.3	28.0	28.4	28.2	28.6	28.2	28.6	28.4
N_2H_4	28.2	28.4	28.2	28.6	28.4	28.9	28.5	28.9	28.5
NaH	25.6	25.8	25.6	25.6	25.5	25.4	25.5	25.4	25.5
NH_3	31.3	31.2	31.3	31.6	31.4	31.9	31.5	31.9	31.5
NH_3HF	30.3	30.2	30.3	30.5	30.3	30.8	30.3	30.8	30.5
NH_3HF	22.0	21.3	21.9	22.1	21.9	22.9	22.2	22.9	22.1
PbH_4	26.4	26.5	26.4	26.5	26.4	26.5	26.4	26.5	26.4
PH_3	29.1	29.0	29.1	29.2	29.0	29.2	29.1	29.3	29.1
RbH	24.6	24.9	24.6	24.7	24.6	24.5	24.6	24.5	24.5
SbH_3	27.5	27.6	27.6	27.7	27.5	27.6	27.6	27.6	27.6
ScH_3	24.0	24.8	24.0	23.9	25.0	24.0	24.1	24.0	24.1
SeH_2	29.9	29.8	30.0	30.0	29.9	30.2	30.0	30.2	30.0
SiH_4	27.4	27.5	27.4	27.5	27.3	27.4	27.4	27.4	27.4
SnH_4	26.6	26.7	26.6	26.7	26.6	26.7	26.6	26.7	26.6
SrH_2	24.5	24.8	24.5	24.6	24.5	24.4	24.5	24.4	24.4
TeH_2	29.2	29.0	29.2	29.3	29.1	29.3	29.3	29.3	29.3
TiH_4	19.4	19.8	19.4	19.3	18.0	19.2	19.2	19.2	19.2
TlH	21.5	21.7	21.5	21.4	21.2	21.0	20.9	21.0	21.0
TlH_3	23.6	24.0	23.6	23.6	23.6	23.9	23.8	23.9	23.8
VH_5	10.8	7.7	10.8	10.8	11.0	10.0	10.0	10.1	10.2
VH_5	15.2	14.9	15.2	15.2	13.0	15.0	15.0	15.0	15.0
ZnH_2	26.7	26.9	26.7	26.7	26.7	26.7	26.6	26.7	26.6
$Zn(CH_3)_2$	31.2	31.3	31.1	31.2	31.2	31.4	31.1	31.4	31.3

3.1.2 Group 2s

Table 4 NMR isotropic shielding constants of various molecules containing 2s elements. Experimental Li-NMR shifts span a range of 10 ppm[30] and Be-NMR shifts a range of 40 ppm (see Ref. 31 and references therein).

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
Be_2F_4	103.6	105.1	101.9	104.0	110.3	107.8	107.8	107.8	105.5
Be_2H_4	79.7	82.5	78.3	79.9	88.5	84.9	84.6	84.9	82.2
Be_4	139.5	137.9	138.7	139.2	145.6	141.4	141.4	141.4	140.6
BeC_2H_6	70.6	72.6	69.2	71.0	81.6	76.4	76.2	76.4	73.0
$BeF_2O_2H_4$	104.6	106.2	103.1	105.3	110.8	108.4	108.3	108.4	106.3
BeH_2	75.4	77.3	73.8	75.4	85.6	81.6	81.2	81.6	78.7
BeS	97.4	98.4	96.0	97.4	113.0	102.2	102.1	102.4	99.6
Li_2	98.6	98.2	98.4	98.5	99.7	99.0	98.9	99.0	98.9
Li_2O	84.3	85.3	83.8	84.4	88.0	84.8	84.7	84.8	84.7
$Li_4C_4H_{12}$	85.0	85.8	84.4	85.0	87.1	85.7	85.4	85.7	85.5
Li_4Cl_4	88.6	89.2	88.1	88.7	90.5	89.4	89.0	89.4	89.3
Li_4H_4	87.2	87.6	86.7	87.1	89.7	88.1	87.6	88.1	87.9
Li_8	101.3	101.3	100.9	101.2	103.5	101.9	101.7	101.9	101.8
$LiBH_4$	90.3	90.9	89.9	90.3	92.0	90.8	90.6	90.8	90.7
LiCl	87.6	88.0	86.9	87.5	91.0	88.0	87.9	88.0	87.8
LiF	87.3	87.9	86.5	87.2	90.3	87.7	87.7	87.7	87.6
LiH	89.2	88.7	88.6	88.9	92.6	89.9	89.6	89.9	89.7
Li_2S	86.2	86.5	85.4	85.9	89.6	86.4	86.3	86.0	86.1
Li_3P	89.7	89.2	89.0	89.5	94.0	90.5	90.3	90.6	90.3

3.1.3 Group 2p

Table 5 NMR isotropic shielding constants of various molecules containing 2p elements. Organic carbon NMR shifts span a range of ca. 230 ppm[29]. Boron covers a range of 250 ppm,[30] nitrogen of more than 800 ppm[32] and up to 1700 ppm,[33] oxygen up to 2000 ppm[34,35] and fluorine of 400 ppm[33].

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
Al_2O_3	291.2	299.0	291.4	295.0	294.8	289.2	289.0	288.6	293.7
Al_2O_3	217.8	229.7	218.1	215.7	212.4	211.5	212.4	211.5	214.7
AlF_3	378.4	390.3	378.7	371.4	372.3	369.4	369.1	369.4	382.8
AtF_3	174.1	228.6	175.1	157.9	169.3	176.3	176.3	176.6	174.4
AtF_3	205.2	256.4	206.3	190.4	201.4	208.8	208.8	209.1	207.1
B_2H_6	72.2	79.3	72.5	75.6	75.4	78.7	78.8	78.7	74.6
$B_3N_3H_6$ (B)	65.7	69.6	65.9	69.5	69.3	72.7	72.8	72.7	68.2
$B_3N_3H_6$ (N)	103.2	115.9	103.7	109.3	108.8	111.8	110.9	111.8	105.8
B_4H_4	−81.6	−83.1	−80.9	−75.0	−75.2	−69.4	−69.5	−69.4	−76.5
BaF_2	−18.1	45.9	−8.5	−37.2	−41.6	−45.1	−39.7	−45.4	−29.4
BaO	−705.6	−844.6	−768.6	−773.7	−781.3	−747.5	−738.3	−748.0	−765.6
Be_2F_4	347.4	360.0	347.4	350.7	356.4	349.3	349.3	349.3	351.6
Be_2F_4	355.5	367.5	355.5	358.8	353.0	348.5	348.5	348.5	357.3
BeC_2H_6	192.6	195.9	192.8	194.6	195.1	195.1	195.3	195.1	193.5
$BeF_2O_2H_4$ (F)	368.7	379.9	368.8	361.8	369.6	360.7	360.4	360.7	374.2
$BeF_2O_2H_4$ (O)	283.0	289.5	283.2	288.5	291.0	287.4	286.5	287.4	283.6
BF_3 (B)	82.2	88.0	82.4	86.0	85.5	88.2	88.2	88.2	84.0
BF_3 (F)	289.0	303.4	289.3	290.4	289.2	289.9	289.9	289.9	292.2
BH_3	−7.8	2.2	−7.3	−2.9	−3.2	2.8	2.0	2.8	−3.8
BH_3CO (B)	157.1	158.9	157.2	158.8	158.9	160.8	160.8	160.8	158.0
BH_3CO (C)	−18.6	−19.5	−17.8	−10.9	−11.8	−8.3	−8.0	−8.3	−14.8
BH_3CO (O)	−47.4	−49.6	−46.6	−40.1	−40.0	−38.3	−38.2	−38.3	−44.8
BH_3NH_3 (B)	116.9	121.6	117.1	119.7	119.5	122.3	122.0	122.3	118.9
BH_3NH_3 (N)	216.2	223.2	216.4	219.1	218.7	221.0	219.9	221.0	217.2
BiF_3	152.7	198.0	153.6	138.5	150.5	149.9	149.9	150.0	157.1
C_2H_2	104.5	106.5	105.0	108.8	108.2	110.7	110.5	110.7	106.9
C_2H_3N (N)	225.4	235.2	225.7	227.5	227.3	229.3	229.1	229.3	226.5
C_2H_3N (C)	53.5	57.8	54.0	58.8	58.6	61.5	61.6	61.5	56.6
C_2H_4	43.4	47.0	44.0	49.1	49.0	52.7	52.5	52.7	46.8
C_2H_6	167.4	172.4	167.7	170.0	169.7	171.4	171.5	171.4	169.2
C_4H_4	204.0	209.1	204.2	205.5	204.9	207.3	206.9	207.3	204.6
C_6H_6	40.0	43.1	40.6	45.8	45.6	49.9	49.8	49.9	43.6
CaF_2	159.9	249.2	209.2	194.2	174.0	158.1	158.1	157.2	174.5
CdF_2	400.6	449.2	401.6	375.6	399.8	383.6	383.3	383.6	398.8
$Cd(CH_3)_2$	185.2	193.0	185.4	186.8	189.0	187.6	187.6	187.6	186.4
CF_4 (C)	35.1	46.3	35.7	41.4	39.5	41.8	41.8	41.8	38.5
CF_4 (F)	216.9	232.9	217.5	225.2	224.4	220.6	220.6	220.6	221.1
CH_2O (C)	−29.4	−23.9	−28.7	−20.5	−21.2	−16.8	−17.0	−16.8	−24.7
CH_2O (O)	−448.6	−453.7	−446.7	−442.1	−440.8	−431.9	−432.6	−431.9	−445.2
CH_2O_2 (C)	83.4	90.1	83.9	87.6	87.2	90.0	90.0	90.0	85.7
CH_2O_2 (O)	21.6	40.9	22.5	28.2	29.0	29.6	29.1	29.6	24.3
CH_3N (N)	−132.2	−131.3	−131.0	−126.0	−125.0	−118.2	−118.9	−118.2	−129.1
CH_3N (C)	1.0	4.7	1.6	8.8	8.3	12.4	12.1	12.4	5.4
CH_4	185.0	187.8	185.2	187.1	186.9	188.5	188.7	188.5	186.1
ClF	629.7	639.6	628.6	612.8	630.2	626.1	626.3	625.4	627.7
ClF_3	−182.6	−98.0	−180.2	−165.5	−165.8	−164.9	−164.6	−164.6	−176.0
ClF_3	21.7	29.9	21.9	31.2	44.5	34.8	35.3	34.9	26.9
CO (C)	−21.9	−25.6	−21.1	−15.8	−15.1	−12.2	−12.2	−12.2	−18.5
CO (O)	−95.8	−100.0	−94.8	−88.0	−89.1	−88.0	−88.0	−88.0	−93.0
CO_2 (C)	47.5	47.1	48.1	53.6	52.4	55.0	55.0	55.0	50.3
CO_2 (O)	199.0	200.3	199.4	201.9	202.1	201.6	201.6	201.6	200.2
$Cr(CO)_6$ (C)	−42.7	−53.0	−41.9	−34.5	−33.7	−30.6	−30.7	−30.6	−38.8
$Cr(CO)_6$ (O)	−103.0	−114.5	−102.0	−95.0	−94.9	−91.1	−91.0	−91.0	−99.5
CrO_3	−1446.0	−1868.7	−1440.3	−1411.2	−1411.7	−1405.6	−1398.7	−1405.3	−1443.0
CS_2	−24.5	−36.6	−23.8	−17.4	−18.0	−12.6	−12.6	−14.6	−19.6
CsF	119.2	179.5	113.7	67.5	29.3	55.7	63.5	55.2	93.3
Cu_2O	582.3	616.2	581.2	582.6	624.7	575.1	579.1	573.8	579.6
CuCN (C)	68.7	55.9	69.3	75.9	76.4	78.0	77.8	77.9	73.2
CuCN (N)	−119.3	−119.0	−118.2	−114.4	−114.2	−108.9	−108.9	−108.7	−117.2
CuF	677.1	637.0	675.1	673.0	731.1	667.0	666.6	665.6	685.2

F_2	−274.9	−246.5	−273.1	−251.6	−255.1	−257.4	−257.4	−257.4	−272.9
$Fe(CO)_5$ (C)	−45.6	−53.6	−44.8	−37.1	−36.9	−32.9	−33.0	−32.9	−41.4
$Fe(CO)_5$ (C)	−60.4	−73.4	−59.5	−51.3	−51.6	−48.0	−48.2	−48.0	−56.2
$Fe(CO)_5$ (O)	−103.6	−106.5	−102.6	−95.8	−95.0	−90.9	−91.0	−90.9	−100.1
$Fe(CO)_5$ (O)	−137.2	−160.6	−136.2	−129.0	−129.4	−125.9	−126.1	−125.9	−133.6
Ferrocene	99.8	107.5	100.3	104.3	104.0	107.7	107.2	107.6	102.4
GaF	72.4	118.9	73.9	47.4	54.8	61.6	61.6	61.3	78.1
GeF_4	298.0	328.2	298.5	291.8	296.0	292.3	292.3	292.4	301.2
GeO	−424.7	−430.9	−422.5	−425.6	−424.9	−420.8	−420.8	−420.6	−432.8
GeO_2	−51.4	−59.5	−50.2	−48.0	−46.2	−49.7	−49.7	−49.6	−52.4
H_2CO_3 (C)	13.6	16.4	14.2	20.5	19.4	22.8	22.6	22.8	17.4
H_2CO_3 (O)	12.2	13.4	12.8	20.6	22.7	22.0	21.8	22.0	16.4
H_2CO_3 (O)	147.1	155.9	147.4	156.2	156.8	155.9	155.0	155.9	151.0
H_2O	318.4	319.9	319.0	327.6	330.2	325.6	324.5	325.6	318.8
H_2O_2	84.1	98.9	84.8	89.4	90.1	91.1	91.3	91.1	85.4
H_2SO_4 (O)	19.5	36.1	20.3	32.0	30.3	28.7	28.0	29.2	23.7
H_2SO_4 (O)	81.5	93.6	82.3	94.1	90.5	89.0	89.1	88.7	85.3
H_3PO_4	193.6	204.8	194.2	203.5	199.3	198.6	198.0	198.6	197.3
$H_3\ PO_4$	150.1	163.8	150.7	156.6	158.5	153.4	152.6	153.1	151.7
$CHBr_3$	54.5	70.1	54.9	59.2	58.9	61.0	60.8	61.0	57.4
HCN (C)	67.1	66.6	67.7	72.8	71.8	74.2	74.1	74.2	69.7
HCN (N)	−52.8	−55.4	−51.9	−46.8	−46.2	−43.7	−43.6	−43.7	−49.7
HCP	10.3	9.6	11.0	16.0	15.6	21.5	21.1	21.2	13.9
HF	403.4	405.4	403.6	404.9	408.2	404.6	404.2	404.6	409.3
HfO	−724.8	−780.6	−722.4	−707.7	−713.1	−701.0	−701.5	−701.1	−722.2
HfO_2	−455.8	−522.3	−453.9	−443.6	−448.9	−443.8	−437.9	−445.0	−457.5
HgF_2	359.4	423.9	360.0	337.1	362.7	343.1	343.5	343.0	358.4
$Hg(CH_3)_2$	175.3	183.5	175.5	177.2	179.5	177.8	177.9	177.8	176.7
HNC (N)	85.6	84.4	86.2	92.4	90.3	93.1	92.3	93.1	88.1
HNC (C)	1.3	−1.2	2.0	6.7	7.9	11.3	10.5	11.3	5.0
HNO (O)	−2126.4	−2294.5	−2119.3	−2109.5	−2095.3	−2081.1	−2090.6	−2081.1	−2121.8
HNO (N)	−1052.9	−1128.0	−1048.4	−1033.8	−1020.9	−1012.3	−1017.8	−1012.3	−1041.9
HNO_2 (N)	−121.2	−146.4	−120.3	−108.4	−109.8	−106.1	−106.4	−106.1	−115.3
HNO_2 (O)	−375.0	−392.8	−373.2	−362.3	−361.0	−355.9	−356.1	−355.9	−369.7
HNO_3 (N)	−98.9	−116.7	−98.0	−87.8	−89.2	−85.9	−85.9	−85.9	−93.8
HNO_3 (O)	−199.5	−217.7	−198.5	−183.6	−182.7	−181.8	−182.1	−181.8	−192.6
HNO_3 (O)	−101.0	−99.9	−100.1	−89.8	−87.1	−88.2	−88.9	−88.2	−97.0
HNO_3 (O)	−194.3	−222.5	−193.1	−177.1	−179.0	−175.7	−176.1	−175.7	−187.2
KF	296.2	313.6	284.9	315.3	263.6	286.1	286.1	285.6	314.5
LaF_3	−78.6	−17.6	−68.4	−56.0	−185.2	−100.4	−94.8	−100.5	−89.7
Li_2O	159.9	165.9	159.7	164.5	215.3	192.5	185.7	192.5	180.2
$Li_4C_4H_{12}$	193.6	197.8	193.8	195.8	196.7	198.1	197.0	198.1	195.1
$LiBH_4$	142.4	145.0	142.5	144.2	145.5	146.4	146.5	146.4	144.6
LiF	341.9	361.3	342.6	328.3	332.1	321.5	324.7	321.5	347.2
MgF_2	427.9	434.6	428.0	406.5	440.7	416.2	416.2	416.0	427.9
$Mo(CO)_6$ (C)	−36.3	−43.2	−35.5	−28.0	−28.1	−24.5	−24.5	−24.5	−32.5
$Mo(CO)_6$ (O)	−99.3	−107.4	−98.3	−91.1	−90.3	−87.6	−87.2	−87.6	−96.0
MoO_3	−736.1	−880.2	−733.0	−720.0	−718.1	−719.7	−713.2	−719.6	−741.5
N_2	−98.6	−106.8	−97.4	−92.6	−90.2	−87.3	−87.3	−87.3	−95.6
N_2H_2	−380.2	−386.6	−378.6	−363.6	−362.6	−355.1	−357.4	−355.1	−371.5
N_2H_4	185.4	193.6	185.8	188.9	188.6	191.2	190.3	191.2	186.0
N_4	206.2	213.1	206.6	208.9	208.4	210.1	210.1	210.1	207.7
Na_2O	326.4	385.3	329.5	315.0	341.1	342.5	342.5	341.7	334.7
Na_3N	−135.6	−340.3	−130.7	−147.9	−123.8	−118.8	−118.8	−118.3	−131.9
NaF	445.8	455.9	447.6	415.1	402.8	414.1	414.1	414.0	445.2
NbO_2F (O)	−761.1	−866.1	−758.0	−745.4	−744.8	−745.2	−738.9	−745.1	−767.2
NbO_2F (F)	53.9	102.3	55.0	43.2	49.8	47.4	48.9	47.3	50.3
Ne_2	550.1	550.7	550.0	552.1	552.5	551.4	551.4	551.4	551.1
NF_3 (N)	−197.8	−179.5	−196.5	−186.2	−186.0	−183.2	−183.2	−183.2	−192.7
NF_3 (F)	−30.7	3.2	−29.9	−5.0	−10.0	−17.1	−17.1	−17.1	−22.5
NH_3	254.8	256.3	255.0	260.9	261.0	261.7	259.7	261.7	254.8
NH_4F (N)	242.3	245.3	242.5	245.5	244.6	246.4	245.0	246.4	242.6
NH_4F (F)	365.1	370.8	364.8	380.2	380.5	378.5	374.9	378.5	385.6
$Ni(CO)_4$ (C)	−29.3	−33.8	−28.5	−21.2	−21.7	−17.2	−17.4	−17.2	−25.1
$Ni(CO)_4$ (O)	−90.7	−97.4	−89.8	−83.0	−82.6	−78.4	−78.5	−78.4	−87.0
OF_2 (O)	−700.7	−624.7	−698.6	−660.4	−660.1	−669.3	−669.3	−669.3	−691.5
OF_2 (F)	−122.8	−85.6	−121.6	−97.1	−101.2	−104.3	−104.3	−104.3	−117.0

$Os(CO)_5$ (C)	−48.9	−50.6	−48.1	−40.2	−40.1	−36.0	−35.8	−36.0	−44.8
$Os(CO)_5$ (C)	−51.1	−53.6	−50.2	−42.1	−43.3	−39.6	−39.5	−39.6	−47.1
$Os(CO)_5$ (O)	−131.3	−119.2	−119.2	−119.2	−119.2	−119.2	−119.2	−119.2	−128.6
$Os(CO)_5$ (O)	−124.0	−130.0	−123.1	−116.1	−115.8	−113.8	−113.3	−113.8	−121.3
OsO_3	−766.4	−739.5	−739.5	−739.5	−739.5	−739.5	−739.5	−739.5	−759.3
OsO_4	−553.7	−699.1	−552.4	−537.3	−533.2	−537.7	−532.7	−537.7	−553.8
PbO	−679.2	−726.8	−676.7	−698.1	−694.3	−688.7	−688.7	−688.5	−706.2
PbO_2	−512.7	−603.2	−511.0	−513.3	−507.2	−518.7	−518.8	−517.7	−530.8
$Pd(CO)_4$ (C)	−27.2	−29.5	−26.5	−19.2	−19.6	−16.1	−16.4	−16.1	−23.4
$Pd(CO)_4$ (O)	−100.6	−104.3	−99.6	−93.8	−92.1	−90.6	−90.6	−90.6	−97.7
PF_3	159.0	169.1	169.1	169.1	169.1	169.1	169.1	169.1	166.4
PF_5	184.4	204.6	185.2	191.5	189.4	185.9	185.9	185.9	190.9
PF_5	194.6	215.3	195.6	201.5	198.7	196.0	195.9	196.0	197.6
PoF_2	364.0	426.4	364.8	347.4	360.4	369.1	369.1	369.2	374.2
PoF_6	−377.2	−220.4	−374.5	−385.3	−376.3	−391.1	−391.1	−390.2	−395.3
PoO_2	−1261.5	−1553.8	−1256.8	−1263.1	−1245.3	−1258.9	−1258.9	−1257.7	−1291.1
$Pt(CO)_4$ (C)	−27.7	−30.7	−26.9	−19.6	−20.4	−16.4	−16.4	−16.4	−23.5
$Pt(CO)_4$ (O)	−97.1	−101.1	−96.2	−89.8	−89.0	−86.9	−86.7	−86.9	−94.3
PtO_2	−256.1	−246.0	−255.3	−247.1	−243.1	−240.8	−246.3	−240.9	−251.9
RbF	243.6	287.5	256.3	238.2	220.2	213.7	219.3	212.8	247.4
Re_2O_7	−10.2	20.9	−9.7	1.7	−0.1	2.5	1.8	2.4	−7.7
Re_2O_7	−549.8	−657.4	−548.3	−534.7	−532.3	−532.9	−528.0	−533.0	−550.2
RnF_2	142.9	206.3	144.9	108.5	131.9	134.1	134.1	135.0	128.9
$Ru(CO)_5$ (C)	−48.7	−51.4	−47.8	−40.0	−39.6	−35.5	−35.7	−35.6	−44.8
$Ru(CO)_5$ (C)	−55.1	−59.4	−54.2	−46.1	−46.9	−43.3	−43.4	−43.3	−51.2
$Ru(CO)_5$ (O)	−130.9	−131.5	−129.8	−123.0	−121.7	−118.0	−117.8	−118.0	−128.1
$Ru(CO)_5$ (O)	−135.4	−144.3	−134.3	−127.5	−126.9	−124.8	−124.6	−124.7	−132.8
RuO_2	−475.8	−581.5	−474.0	−465.6	−457.3	−455.3	−456.6	−455.2	−470.7
RuO_4	−789.8	−1077.1	−787.0	−770.1	−768.3	−774.0	−765.4	−773.9	−796.1
SbF_3	165.8	206.9	167.1	156.5	164.2	166.6	166.6	166.6	173.2
ScF_3	−67.5	−0.6	−66.0	−72.8	−71.3	−73.3	−65.5	−74.0	−70.1
SeO_2	−673.1	−751.3	−670.7	−660.7	−656.7	−654.9	−654.9	−655.1	−674.0
SF_2	292.7	328.4	293.2	306.0	306.3	304.6	304.9	305.1	303.1
SF_4	−9.6	23.2	−8.1	9.1	6.8	5.5	5.7	6.3	−1.5
SF_4	35.6	72.6	36.7	51.1	52.5	48.0	48.6	47.7	42.1
SF_6	6.7	38.0	7.7	16.8	18.5	14.4	14.4	14.5	11.2
SiF_4	324.4	338.3	325.1	325.5	323.0	320.2	319.9	320.2	328.5
SiO_2	172.2	180.4	172.3	162.4	173.3	171.1	170.9	170.9	170.5
SnO	−623.0	−649.9	−618.0	−636.2	−628.1	−624.6	−624.6	−624.5	−640.3
SnO_2	−310.2	−360.2	−307.2	−311.8	−305.1	−311.5	−311.5	−311.5	−319.5
SrF_2	111.6	154.7	113.4	84.3	84.2	93.0	96.5	92.1	109.1
SrO	−402.5	−522.7	−400.5	−374.8	−338.1	−393.2	−389.2	−394.7	−402.5
TaF_3	−80.0	−22.1	−78.4	−81.5	−80.1	−81.3	−77.8	−81.4	−81.4
TaO_2F (F)	78.7	112.8	79.8	68.9	70.4	71.2	73.8	70.8	75.0
TaO_2F (O)	−726.6	−756.0	−723.8	−713.2	−721.8	−715.0	−703.8	−715.8	−737.9
Tc_2O_7	−124.3	−84.6	−123.3	−109.5	−112.7	−113.3	−110.3	−113.6	−125.5
Tc_2O_7	−750.5	−947.3	−747.8	−731.7	−729.5	−732.4	−725.3	−732.4	−754.7
TcO_3F (F)	88.3	149.4	89.0	83.7	88.6	88.2	87.4	88.2	88.7
TcO_3F (O)	−746.9	−949.5	−744.0	−727.9	−726.1	−730.5	−722.9	−730.5	−752.3
TeO_2	−896.8	−1029.1	−893.2	−897.1	−883.1	−888.2	−888.2	−888.3	−913.3
$Ti(CO)_4$ (C)	−428.2	−630.9	−426.0	−411.1	−411.7	−400.1	−400.8	−399.4	−422.4
$Ti(CO)_4$ (O)	−1225.2	−1973.1	−1221.1	−1214.4	−1219.9	−1207.5	−1207.8	−1205.2	−1229.6
TiF_4	−179.6	−147.6	−177.9	−177.9	−176.0	−178.6	−176.4	−178.6	−180.5
TiO_2	−829.5	−964.3	−826.6	−809.5	−814.6	−806.1	−803.5	−806.4	−829.1
$W(CO)_6$ (C)	−32.8	−38.4	−32.0	−24.3	−24.3	−21.2	−21.2	−21.2	−28.8
$W(CO)_6$ (O)	−90.9	−97.3	−90.0	−83.6	−82.1	−78.9	−78.5	−78.8	−87.2
WO_3	−943.9	−969.9	−940.6	−931.4	−938.8	−935.2	−916.7	−936.0	−966.5
XeF_2	256.3	301.0	256.7	234.7	261.0	251.3	251.3	251.4	248.6
XeF_4	42.9	89.8	43.9	38.5	56.3	48.2	48.2	48.3	43.5
$XeOF_4$ (O)	−398.3	−407.5	−397.8	−397.0	−376.7	−395.7	−395.7	−395.8	−413.3
$XeOF_4$ (F)	−139.5	−76.9	−137.4	−137.5	−125.6	−132.2	−132.2	−132.2	−139.0
YF	−200.0	−131.9	−197.6	−200.2	−199.9	−208.2	−197.0	−208.3	−205.2
YF_3	25.6	74.6	27.0	17.4	17.5	11.3	20.7	11.4	20.7
ZnF_2	412.4	443.2	412.8	391.5	413.7	402.1	402.1	402.0	416.7
$Zn(CH_3)_2$	184.4	191.6	184.7	186.5	188.0	187.9	188.1	187.9	186.4
ZrO	−778.4	−892.1	−775.4	−760.6	−762.9	−754.3	−753.6	−753.9	−776.9
ZrO_2	−734.5	−806.1	−731.6	−724.4	−730.0	−721.3	−716.5	−721.5	−741.5

3.1.4 Group 3s

Table 6 NMR isotropic shielding constants of various molecules containing 3s elements. Mg-NMR chemical shifts show a range of 200 ppm.[36]

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
Mg_4	707.2	710.1	707.2	707.5	701.8	705.5	705.5	707.1	706.7
$MgCl_2$	496.9	507.1	497.2	498.3	498.7	492.8	492.8	498.9	496.0
MgF_2	538.2	550.0	538.4	539.8	536.1	534.4	534.4	540.0	537.7
MgH_2	426.1	437.3	426.5	427.8	440.5	425.2	424.4	428.0	424.5
Na_2	610.7	608.3	610.6	611.2	609.8	608.2	608.2	610.9	610.4
Na_2O	584.7	574.0	584.4	586.3	582.6	581.2	581.2	582.9	582.3
Na_2S	567.6	562.6	567.5	568.7	565.9	564.3	564.2	567.2	566.4
Na_3N	588.6	582.1	588.3	590.3	587.8	584.5	584.5	589.3	588.3
Na_3P	581.9	573.1	581.7	583.4	581.3	579.6	579.7	582.5	581.8
Na_3P	582.0	573.2	581.8	583.5	581.4	579.7	579.7	582.6	581.9
Na_3P	582.5	573.7	582.3	584.0	581.9	580.2	580.2	583.1	582.3
NaCl	570.1	569.9	570.1	570.7	568.8	567.7	567.7	569.9	569.1
NaF	580.1	580.3	580.0	580.3	579.0	577.3	577.3	579.7	578.5
NaH	577.3	572.4	577.2	578.1	576.6	575.6	575.7	577.6	577.0

3.1.5 Group 3p

Table 7 NMR isotropic shielding constants of various molecules containing 3p elements. The range of the Al-NMR shifts is ca. 200 ppm[37,38], silicon shows a range of 959 ppm[39,40], phosphorus of roughly 500 ppm[41,42], sulfur of 1000 ppm[43,44] and chlorine of more than 1000 ppm[45].

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
AgCl	960.7	1087.1	961.1	941.5	957.1	922.5	935.2	925.8	925.1
Al_2O_3	478.6	477.6	479.0	485.0	477.4	483.2	482.1	481.8	478.7
Al_2S_3 (Al)	379.3	377.3	379.9	386.2	377.9	383.5	383.4	384.3	381.0
Al_2S_3 (S)	647.5	693.0	648.5	647.9	642.8	641.7	642.5	651.1	649.0
Al_2S_3 (S)	590.5	633.9	591.3	578.0	581.4	576.2	577.6	585.5	583.4
$AlCl_3$ (Al)	398.0	413.2	398.4	405.5	396.5	403.8	404.2	403.7	400.3
$AlCl_3$ (Cl)	877.4	912.2	878.2	877.5	871.7	870.0	870.1	875.0	874.4
AlF_3	492.9	509.0	492.9	498.6	492.1	497.1	497.4	496.0	493.1
AlH_3	254.7	281.7	255.6	262.4	253.6	260.0	259.5	260.7	256.8
Ar_2	1240.6	1241.0	1240.5	1241.9	1237.3	1241.4	1241.3	1242.4	1248.5
As_4S_4	721.6	772.2	722.6	730.2	720.9	724.9	725.2	733.9	731.4
$AsCl_3$	480.0	551.3	480.5	484.5	482.9	484.2	484.4	499.3	496.3
AtCl	1214.8	1268.5	1215.3	1223.3	1217.1	1219.3	1218.5	1220.2	1219.1
AuCl	812.1	995.7	812.7	808.3	842.5	774.1	789.6	780.4	779.8
BaS	−236.3	−397.3	−303.7	−285.2	−264.1	−339.6	−332.6	−315.2	−319.3
BeS	1073.2	1038.3	1074.1	1072.0	1045.7	1074.2	1074.3	1073.3	1074.5
BrCl	692.0	742.2	692.1	704.0	688.7	688.9	688.0	700.5	698.1
$CaCl_2$	794.2	904.4	863.7	877.2	849.3	791.8	792.1	796.6	795.7
Cd_2Cl_2	817.2	894.0	817.8	805.3	832.0	796.4	796.8	802.8	797.5
Cl_2	417.8	462.4	419.5	424.8	417.7	411.1	411.8	428.5	424.7
ClF	−846.1	−782.6	−839.2	−736.5	−793.8	−842.8	−842.9	−794.8	−819.6
ClF_3	−955.9	−752.8	−948.3	−892.9	−943.4	−977.4	−977.8	−925.6	−944.5
CS_2	472.0	479.5	473.4	476.2	467.6	463.6	463.5	478.2	475.3
Cu_2S	920.8	984.1	921.4	932.6	935.5	922.5	927.6	926.5	924.0
CuCl	1123.3	1161.0	1123.9	1127.5	1151.4	1120.5	1123.5	1119.9	1118.8
GaCl	436.0	498.7	437.9	421.8	419.8	412.5	412.6	427.1	424.7
$GaCl_3$	740.8	815.7	742.0	740.2	737.0	736.4	736.3	744.2	742.9
$GeCl_4$	565.9	652.6	567.3	554.0	563.0	563.8	563.8	576.2	573.3
H_2SO_4	117.8	120.5	122.7	142.9	110.6	106.4	105.1	125.5	121.2
H_3PO_4	260.7	279.3	263.1	275.5	256.0	251.8	252.3	264.9	256.6
HCl	926.5	934.9	928.0	929.6	921.0	915.6	919.8	923.0	921.4
HCP	323.2	321.4	324.1	321.5	317.6	312.2	311.5	326.1	318.3
Hg_2Cl_2	695.4	801.9	696.2	681.1	713.9	671.0	673.4	680.5	679.8
H_2S	690.7	699.4	693.0	695.7	683.8	674.5	678.6	685.2	682.8
H_2S_2	525.7	552.3	527.9	534.8	520.6	513.2	515.7	526.7	523.4
ICl	1109.7	1151.3	1107.8	1111.3	1105.8	1108.0	1107.1	1109.1	1109.0
InCl	493.1	570.0	496.7	471.9	475.5	461.4	461.7	475.0	472.5
$InCl_3$	810.6	893.7	812.2	804.3	803.5	798.6	798.8	804.9	804.1
K_2S	744.7	837.0	735.1	753.2	743.5	774.9	774.8	789.4	784.4
K_3P	386.0	377.2	397.2	344.3	365.3	405.9	405.7	422.4	416.0
KCl	1006.6	1013.9	990.8	1021.4	984.5	994.5	994.6	996.6	996.0
$LaCl_3$	352.8	435.6	360.3	360.8	225.6	311.4	315.9	327.0	324.0
Li_4Cl_4	995.2	1015.7	995.1	997.2	1000.7	1015.4	1001.2	1025.2	1022.5
LiCl	1017.9	1032.5	1018.0	1000.3	1023.8	999.7	1003.1	1003.5	1002.7
Li_2S	864.5	869.3	863.6	866.8	915.6	891.7	889.1	904.2	901.0
$MgCl_2$	1062.7	1078.8	1062.9	1053.1	1081.9	1051.5	1051.8	1051.6	1052.2
Na_2S	1031.3	1058.5	1032.1	1029.7	1043.9	1036.3	1036.4	1041.6	1039.9
Na_3P	561.0	582.1	564.3	545.4	559.9	553.1	553.1	562.5	557.7
NaCl	1116.0	1128.9	1116.9	1093.5	1096.2	1087.8	1088.0	1086.4	1087.1
P_2	−337.5	−373.3	−335.2	−344.3	−350.9	−366.4	−365.6	−342.0	−358.6
PF_3	135.8	165.2	137.9	143.7	126.5	120.6	121.0	136.7	129.8
PF_5	324.0	353.6	326.0	336.4	318.9	315.8	316.1	327.1	319.3
PH_3	567.8	577.1	569.1	575.3	563.9	558.8	559.7	567.6	562.7
Li_3P	520.1	500.8	519.3	519.0	569.8	535.1	540.6	546.8	542.3
$PoCl_4$	467.6	550.8	469.2	460.3	457.0	449.7	450.1	465.7	462.0
$PoCl_4$	469.4	551.8	471.0	461.3	457.9	450.1	450.5	466.1	462.4
S_5	5.8	43.9	8.4	18.4	2.6	−7.0	−6.7	18.3	12.1
S_5	−86.3	−64.4	−84.0	−83.4	−92.1	−106.0	−105.6	−79.2	−85.7
S_5	−181.5	−184.9	−179.1	−173.4	−183.1	−195.4	−194.5	−166.1	−173.1
$ScCl_3$	314.5	416.7	316.1	309.1	305.8	285.0	289.3	302.2	298.4

SF_2	−1172.5	−1093.0	−1163.5	−1089.4	−1151.0	−1191.9	−1190.9	−1138.5	−1156.6
SF_4	−105.7	−54.4	−101.4	−91.5	−117.5	−130.8	−130.7	−102.7	−106.2
SF_6	206.7	250.3	210.8	226.3	198.9	193.9	193.0	213.1	208.2
$SiCl_4$ (Si)	311.9	330.2	313.5	321.5	307.8	309.4	309.8	316.6	309.4
$SiCl_4$ (Cl)	684.5	732.1	686.0	696.5	682.1	682.8	682.7	692.4	690.7
SiF_4	429.8	451.2	431.2	438.6	428.2	426.8	427.1	432.6	427.5
SiH_4	432.7	445.0	434.1	444.3	430.4	430.0	429.7	435.8	430.6
SiO_2	326.0	323.1	327.3	334.4	326.2	322.2	322.0	330.1	324.1
SiS_2 (Si)	192.6	180.5	194.0	199.5	190.1	188.0	187.9	197.4	190.0
SiS_2 (S)	565.7	594.6	565.9	551.2	556.9	553.4	553.8	563.4	561.4
SrS	361.3	303.4	363.4	390.6	416.7	344.9	345.7	355.2	353.3
$TiCl_4$	39.9	56.7	42.3	39.0	32.8	8.2	8.9	33.8	28.1
TiS_2	−891.9	−1124.0	−888.2	−889.6	−898.9	−937.0	−933.8	−893.5	−905.4
TlCl	471.8	564.6	474.9	447.2	451.0	436.6	436.8	452.4	448.1
$TlCl_3$	550.5	694.0	551.9	545.3	541.7	527.2	527.5	541.8	538.8
$ZnCl_2$	947.4	1005.0	947.9	940.9	949.8	941.7	941.9	946.0	946.1

3.1.6 Group 4s

Table 8 NMR isotropic shielding constants of various molecules containing 4s elements. Calcium shows NMR shifts from -40 ppm for oxygen to 30 ppm for nitrogen complexes. [46]

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
Ca_4	1309.1	1423.1	1399.6	1416.5	1394.4	1361.7	1361.7	1360.6	1356.3
$CaCl_2$	989.9	1104.9	1065.2	1085.5	1065.4	1018.1	1018.6	1016.3	1015.5
CaF_2	1100.8	1194.6	1158.2	1171.5	1146.9	1122.0	1122.0	1117.8	1114.9
CaH_2	824.9	922.7	890.4	907.3	899.8	857.1	861.7	853.4	854.4
K_2	1292.8	1284.0	1291.3	1293.0	1289.8	1295.6	1295.6	1292.6	1290.7
K_2S	1262.9	1241.1	1252.2	1262.1	1257.8	1272.9	1273.0	1262.5	1262.0
K_3P	1265.5	1240.0	1257.6	1266.0	1261.4	1277.0	1277.0	1264.8	1263.0
KBr	1253.2	1248.8	1245.2	1250.7	1249.0	1260.5	1260.5	1253.0	1252.7
KCl	1257.9	1253.9	1249.9	1254.7	1253.0	1263.4	1263.5	1258.8	1259.4
KF	1289.0	1282.7	1278.8	1284.8	1284.0	1295.9	1295.9	1292.4	1290.8
KH	1247.3	1230.8	1240.4	1245.4	1244.8	1247.1	1248.7	1248.0	1246.9
KI	1249.3	1244.8	1242.2	1247.5	1245.9	1254.9	1254.9	1249.2	1249.8

3.1.7 Group 3d

Table 9 NMR isotropic shielding constants of various molecules containing 3d elements. The range of the NMR shifts is taken from Ref. 47, 48, 49, 50 and 51 (and references therein).

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s	Range
$Cr(CO)_6$	−547.2	−904.3	−545.8	−530.4	−499.6	−452.5	−460.4	−458.8	−513.5	1800
CrO_3	−3477.8	−4780.2	−3474.2	−3461.9	−3377.6	−3298.1	−3299.3	−3301.4	−3414.8	1800
Cu_2	2130.3	2240.1	2132.2	2157.4	2085.5	2138.3	2135.4	2151.1	2145.4	980
Cu_2	−753.0	35.7	−743.4	−792.4	−974.1	−649.6	−653.4	−624.8	−655.2	980
Cu_2S	518.8	1119.5	525.1	497.9	407.5	567.5	563.3	586.4	570.5	980
CuCl	1141.0	1468.2	1147.7	1085.0	995.7	1169.6	1165.8	1190.6	1183.1	980
CuCN	1222.8	1469.2	1224.2	1195.5	1156.5	1233.2	1234.0	1252.9	1241.9	980
CuF	−37.0	603.6	−17.4	−197.4	−388.8	44.3	45.5	70.0	41.9	980
CuH	1444.0	1656.5	1448.5	1391.5	1314.3	1474.1	1474.3	1484.5	1472.7	980
$Fe(CO)_5$	−1859.1	−2854.2	−1856.8	−1835.4	−1786.3	−1764.5	−1764.6	−1761.1	−1818.9	12000
Ferrocene	−2485.8	−4718.8	−2483.5	−2480.6	−2435.3	−2369.2	−2381.1	−2364.7	−2447.2	12000
$Ni(CO)_4$	−1636.6	−2029.4	−1634.5	−1603.8	−1552.3	−1507.0	−1507.2	−1530.2	−1594.2	1196
$ScCl_3$	175.2	357.4	176.2	176.6	192.0	211.8	218.6	197.2	180.1	290
ScF_3	633.9	759.6	634.8	633.9	641.4	649.6	652.5	645.6	636.8	290
ScH_3	−450.2	−268.3	−448.9	−447.1	−410.8	−400.4	−396.8	−418.7	−438.6	290
$TiCl_4$	−1000.5	−925.2	−999.2	−997.7	−974.9	−924.5	−920.4	−933.9	−983.4	2500
$Ti(CO)_4$	−6517.4	−10816.7	−6509.0	−6548.4	−6480.3	−6307.4	−6309.1	−6324.0	−6479.2	2500
TiF_4	−72.0	65.6	−71.0	−72.1	−62.4	−40.4	−35.2	−37.9	−64.7	2500
TiH_4	−2806.3	−2643.4	−2803.9	−2799.4	−2715.7	−2692.7	−2693.4	−2705.3	−2774.1	2500
TiO_2	−356.3	−319.0	−355.2	−352.2	−340.1	−304.9	−301.0	−295.5	−338.0	2500
TiS_2	−1813.6	−1900.3	−1811.7	−1809.8	−1769.4	−1719.2	−1710.2	−1714.6	−1786.0	2500
VH_5	−5304.3	−5796.8	−5300.0	−5295.4	−5167.4	−5124.5	−5132.3	−5130.1	−5234.3	6000
Zn_2	2457.3	2470.6	2457.4	2474.0	2466.7	2451.1	2451.1	2459.8	2452.3	6000
$ZnCl_2$	1634.7	1696.1	1635.3	1649.6	1652.5	1626.2	1626.9	1639.7	1632.8	6000
ZnF_2	1644.0	1729.0	1644.1	1645.3	1649.3	1637.6	1638.3	1653.0	1641.0	365
ZnH_2	1577.9	1645.9	1579.1	1589.4	1611.1	1586.8	1582.0	1584.1	1573.8	365
$Zn(CH_3)_2$	1345.3	1436.7	1346.7	1351.5	1379.4	1366.0	1359.4	1353.9	1338.7	365

3.1.8 Group 4p

Table 10 NMR isotropic shielding constants of various molecules containing 4p elements. The NMR shift range of gallium is about 1300 ppm[52], the range of germaniun ca. 1100 ppm[53], of arsenic 700 ppm,[54], selenium of ca. 2000 ppm (see Ref. 55 and references therein) and bromine of 300 ppm[56,57].

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
As_4	2248.8	2323.5	2249.5	2251.8	2241.3	2236.0	2236.0	2262.0	2255.1
As_4S_4	1380.5	1402.4	1380.6	1383.1	1391.2	1375.6	1376.1	1413.8	1400.4
$AsCl_3$	456.3	576.5	456.5	446.7	468.1	431.5	432.2	475.9	458.5
AsH_3	1871.9	1908.7	1872.7	1872.8	1871.1	1854.2	1864.6	1880.4	1872.4
Br_2	1441.8	1576.7	1440.4	1430.6	1450.2	1458.0	1458.0	1456.5	1450.9
BrCl	776.1	904.9	777.8	748.7	806.9	818.2	822.0	809.3	802.1
GaCl	1671.6	1739.9	1672.1	1670.2	1672.5	1667.2	1667.4	1686.8	1673.3
$GaCl_3$	1348.2	1412.8	1348.8	1350.4	1355.0	1372.5	1372.5	1391.5	1376.2
GaF	1941.3	1998.3	1942.0	1935.8	1936.1	1931.4	1931.4	1951.5	1943.1
GaH_3	1045.9	1153.8	1047.6	1047.0	1058.9	1060.2	1061.2	1086.4	1065.6
$GeCl_4$	1143.4	1208.3	1143.7	1126.6	1148.3	1162.9	1162.9	1167.8	1177.9
GeF_4	1418.3	1492.5	1419.2	1417.0	1425.6	1431.6	1431.6	1436.3	1454.4
GeH_4	1614.8	1659.6	1615.4	1617.2	1619.5	1620.6	1623.9	1630.4	1635.4
GeO	901.7	880.4	902.9	902.1	908.4	881.4	881.4	882.5	898.7
GeO_2	1374.8	1304.0	1375.6	1375.4	1389.2	1378.4	1378.4	1372.5	1393.3
HBr	2547.1	2576.0	2548.3	2540.8	2534.1	2525.6	2532.5	2540.3	2536.8
$CHBr_3$	1256.1	1415.0	1256.6	1260.2	1277.2	1299.7	1303.9	1296.7	1292.3
KBr	2907.3	2929.9	2883.7	2962.7	2890.7	2869.5	2869.5	2904.7	2894.7
$PdBr_2$	2498.0	3168.1	2501.8	2493.5	2475.1	2421.4	2468.3	2436.5	2428.8
$PoBr_2$	2163.5	2378.0	2164.3	2162.2	2166.1	2167.3	2167.3	2181.8	2174.0
Kr_2	3289.3	3291.3	3289.2	3290.9	3272.9	3262.6	3262.6	3291.2	3286.8
Se_8	822.4	856.9	822.0	824.6	847.3	891.1	891.1	870.4	869.3
SeH_2	2046.2	2080.3	2047.9	2037.8	2036.2	2035.6	2039.7	2040.2	2037.6
SeO_2	−467.2	−719.5	−466.1	−462.6	−448.0	−415.6	−415.6	−450.3	−453.3

3.1.9 Group 5s

Table 11 NMR isotropic shielding constants of various molecules containing 5s elements. Common strontium compounds in solution show a NMR chemical shift range of ca. 20 ppm. [58]

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
Rb_2	3331.1	3313.6	3330.4	3331.6	3298.2	3311.4	3314.7	3344.4	3335.4
RbF	3339.1	3343.8	3337.9	3335.9	3314.0	3309.2	3309.1	3340.7	3334.8
RbH	3238.5	3216.6	3236.4	3237.8	3211.5	3204.8	3207.2	3237.3	3231.2
Sr_4	3199.2	3278.4	3199.7	3228.5	3276.5	3207.9	3188.8	3211.8	3229.6
SrF_2	3089.8	3143.4	3089.7	3086.9	3100.1	3065.5	3071.3	3081.5	3087.6
SrH_2	2597.5	2619.3	2597.6	2599.7	2642.8	2587.9	2596.9	2590.0	2600.9
SrO	3162.8	3291.1	3162.4	3176.0	3259.4	3150.8	3155.8	3165.9	3190.2
SrS	2989.1	3101.8	2989.1	3019.4	3105.5	2982.4	2989.6	2988.6	3014.3

3.1.10 Group 4d

Table 12 NMR isotropic shielding constants of various molecules containing 4d elements. The range of the NMR shifts is taken from Ref. 47, 48, 59, 60 and 61.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s	Range
Ag_2	4585.5	4593.2	4585.1	4593.2	4526.5	4530.2	4525.3	4592.5	4581.8	2769
AgCl	4175.9	4167.9	4176.6	4188.3	4134.2	4126.0	4115.8	4197.5	4186.8	2769
Cd_2	4848.0	4860.7	4847.8	4850.9	4782.3	4760.8	4760.7	4850.2	4832.9	950
Cd_2Cl_2	3613.0	3642.7	3612.9	3617.2	3555.5	3551.2	3553.8	3612.9	3593.6	950
CdF_2	3856.9	3902.1	3856.2	3849.2	3777.5	3771.6	3777.4	3855.9	3833.1	950
$Cd(CH_3)_2$	3040.4	3111.9	3040.2	3042.5	3008.8	2979.0	2985.8	3035.0	3015.4	950
Mo_2	−4392.5	−9253.5	−4388.6	−4392.2	−3941.3	−4281.7	−4328.8	−4353.5	−4217.9	1700
$Mo(CO)_6$	1253.4	1219.3	1254.7	1270.9	1332.4	1336.0	1257.9	1268.6	1316.0	1700
MoO_3	−1185.8	−1331.7	−1181.3	−1189.9	−972.1	−1161.1	−1137.9	−1208.2	−1131.5	1700
NbO_2F	240.3	312.0	244.1	237.6	392.5	240.6	260.3	215.6	274.1	5000
$PdBr_2$	−3167.6	−4533.9	−3167.2	−3209.8	−2954.2	−3133.8	−3144.3	−3173.0	−3065.5	-
$Pd(CO)_4$	292.4	370.4	294.5	322.7	375.9	352.8	344.5	322.3	369.3	-
$Ru(CO)_5$	200.8	−11.7	203.8	223.8	314.6	275.2	253.4	220.7	280.2	18000
RuO_2	−4042.1	−4911.7	−4027.1	−4013.9	−3716.5	−4063.2	−3941.1	−4157.6	−4029.4	18000
RuO_4	−2548.0	−3094.1	−2546.9	−2538.1	−2303.7	−2440.7	−2471.1	−2507.0	−2409.4	18000
Tc_2O_7	−1849.9	−2233.2	−1848.3	−1846.3	−1607.3	−1841.8	−1848.9	−1854.9	−1812.8	4500
TcO_3F	−1844.4	−2218.2	−1842.6	−1839.5	−1598.0	−1842.4	−1846.2	−1848.3	−1806.0	4500
YF	2926.3	3033.4	2926.6	2914.6	2961.9	2880.2	2876.8	2913.5	2913.6	700
YF_3	2439.0	2589.0	2441.5	2425.8	2467.3	2391.5	2375.9	2415.2	2413.5	700
ZrO	2035.1	−28471.2	2037.1	2039.6	2115.4	2008.8	2017.9	2024.9	2055.7	1000
ZrO_2	1405.4	1622.3	1409.0	1404.7	1511.1	1383.8	1402.9	1384.2	1425.0	1000

3.1.11 Group 5p

Table 13 NMR isotropic shielding constants of various molecules containing 5p elements. The NMR shifts cover a range of 1070 ppm for indium,[52] 2950 ppm for tin,[30,62] 3450 ppm for antimony, 3500 ppm for tellurium,[63] 1200 ppm for iodine[64] and 7000 ppm for xenon[65–68].

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
HI	2859.1	3112.6	2865.9	2817.5	2774.9	2784.6	2784.6	2827.3	2821.2
I_2	−307.4	−12.4	−277.9	−335.5	−301.3	−235.8	−229.3	−294.5	−289.5
ICl	4358.3	4419.1	4362.9	4354.1	4255.1	4232.2	4251.4	4317.5	4306.9
InCl	3487.6	3606.7	3498.3	3479.9	3415.1	3414.1	3414.2	3474.8	3462.8
$InCl_3$	2908.7	3000.8	2918.7	2907.5	2860.9	2877.2	2877.3	2919.7	2910.5
InH	1803.0	2005.8	1839.6	1788.2	1747.8	1771.5	1767.6	1790.3	1780.8
InH_3	2271.5	2445.3	2294.0	2269.4	2229.0	2251.4	2248.7	2284.4	2275.2
KI	5373.4	5406.8	5336.6	5452.1	5274.7	5230.1	5230.1	5349.3	5332.7
SbF_3	2161.7	2380.9	2163.6	2124.7	2079.6	2124.2	2124.2	2122.6	2126.9
SbH_3	3269.2	3337.2	3272.3	3287.5	3193.3	3223.5	3229.5	3257.5	3250.0
SnH_4	3007.8	3087.1	3013.2	3017.0	2947.9	2983.4	2994.7	3015.3	3006.3
SnO	1756.8	1625.9	1766.3	1736.2	1690.1	1716.3	1716.3	1718.5	1703.4
SnO_2	3017.1	2721.1	3022.2	2986.4	2964.8	2974.0	2974.0	3009.6	2993.1
TeH_2	3427.1	3495.0	3433.8	3432.7	3335.0	3320.4	3337.9	3378.9	3367.5
TeO_2	−488.3	−1103.5	−488.4	−502.1	−524.5	−482.0	−482.0	−530.6	−532.3
XeF_2	2064.5	1940.6	2073.4	2328.3	2171.3	2173.6	2173.6	2223.1	2180.3
XeF_4	−739.7	−424.5	−715.1	−544.9	−707.3	−626.7	−626.7	−652.0	−682.1
$XeOF_4$	−474.2	−443.9	−459.6	−418.4	−524.5	−456.9	−456.9	−480.7	−482.5

3.1.12 Group 6s

Table 14 NMR isotropic shielding constants of various molecules containing 6s elements. Cs-NMR shifts span a range of about 50-200 ppm.[69,70]

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
Ba_4	5403.8	5662.5	5319.8	5383.5	5363.4	5246.8	5204.8	5335.0	5338.8
BaF_2	5580.5	5665.6	5581.2	5578.3	5484.2	5437.8	5452.1	5573.3	5555.9
BaH_2	4531.0	4614.7	4519.9	4534.6	4518.4	4387.8	4407.6	4509.7	4491.9
BaO	5427.0	5671.4	5439.9	5461.8	5446.8	5303.0	5308.6	5463.4	5425.3
BaS	4931.2	5200.3	4921.0	4944.6	4978.1	4790.8	4807.1	4936.8	4900.8
Cs_2	5845.2	5814.6	5844.2	5845.9	5709.1	5707.6	5711.4	5847.6	5830.7
CsF	5882.7	5908.7	5886.2	5882.3	5742.6	5729.4	5733.5	5882.7	5854.7
CsH	5672.4	5658.8	5675.6	5679.5	5542.7	5521.0	5528.0	5672.6	5648.3

3.1.13 Group 5d

Table 15 NMR isotropic shielding constants of various molecules containing 5d elements. The range of the NMR shifts is taken from Ref. 47, 48, 71 and 72.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s	Range
Au_2	9723.2	9809.3	9723.5	9752.5	9172.1	9194.4	9156.6	9753.2	9706.7	-
AuCl	8516.6	8567.5	8516.5	8526.7	7915.1	8048.2	7970.3	8609.2	8553.8	-
HfO	6305.6	6732.0	6306.4	6316.2	6295.7	6016.7	6014.9	6323.5	6317.4	-
HfO_2	4644.6	5294.7	4650.3	4638.7	4769.4	4370.4	4377.7	4623.6	4629.7	-
Hg_2	10518.9	10532.7	10518.3	10529.6	10007.0	9909.4	9909.3	10500.3	10453.7	3510
Hg_2Cl_2	7974.9	7968.0	7974.5	7992.0	7531.6	7450.4	7443.9	7948.2	7915.4	3510
HgF_2	8040.4	8089.6	8040.2	8042.3	7551.4	7464.9	7447.1	8053.5	7972.1	3510
$Hg(CH_3)_2$	6435.2	6523.4	6436.1	6441.4	6087.2	5935.8	5902.2	6389.6	6370.0	3510
$LaCl_3$	3729.4	4001.3	3744.4	3716.4	3025.7	3611.9	3645.6	3717.1	3696.6	1700
LaF_3	4849.9	5043.4	4871.6	4843.9	4323.3	4735.7	4788.3	4836.9	4830.0	1700
LaH_3	2271.4	2575.0	2268.2	2239.6	1683.5	2199.5	2199.3	2269.5	2255.4	1700
$Os(CO)_5$	3115.7	3076.5	3119.1	3150.8	3137.7	2983.8	2783.3	3212.0	3252.7	3500
OsO_3	−5493.8	−6066.2	−5488.7	−5431.9	−4970.9	−5863.1	−5824.9	−5511.1	−5566.9	3500
OsO_4	−1617.5	−1991.8	−1613.0	−1606.1	−1324.7	−1852.3	−1975.8	−1519.2	−1548.5	3500
$Pt(CO)_4$	3097.7	3220.1	3099.5	3144.7	3064.9	2866.2	2684.3	3172.6	3200.2	13000
PtO_2	−3311.7	−4854.7	−3297.5	−3293.4	−3101.0	−3836.3	−3660.2	−3401.9	−3481.6	13000
Re_2O_7	−478.2	−651.4	−478.9	−473.4	−223.4	−850.6	−898.9	−432.4	−498.6	7000
TaF_3	−5215.6	−7371.5	−5206.4	−5042.1	−4182.6	−5617.7	−5387.2	−5394.9	−5378.6	9000
TaO_2F	1410.0	1865.0	1414.4	1416.5	1616.2	1087.6	1102.6	1413.3	1386.8	9000
$W(CO)_6$	4515.4	4632.9	4517.6	4540.2	4411.0	4439.5	4155.9	4613.3	4659.6	11500
WO_3	−2138.8	−2040.2	−2134.3	−2135.6	−1777.3	−2426.2	−2400.6	−2122.5	−2155.4	11500

3.1.14 Group 6p

Table 16 NMR isotropic shielding constants of various molecules containing 6p elements. Thallium shows a range of 5500 ppm.[52], lead of 4750 ppm[62]. Only a limited amount of data on Bi-NMR is available.[73,74]

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
At_2	4691.7	5243.9	4675.2	4561.8	3857.7	3975.1	3975.1	4521.6	4516.3
AtCl	−3156.6	−2741.3	−3167.2	−3300.8	−3957.5	−3460.2	−3445.7	−3183.9	−3138.2
AtF_3	−7551.9	−7391.1	−7561.3	−7328.5	−8159.8	−7592.0	−7592.0	−7478.7	−7469.6
BiF_3	4865.3	5354.1	4874.2	4785.5	4146.2	4262.6	4262.6	4696.3	4811.4
BiH_3	6663.7	6790.4	6668.7	6673.8	6008.9	6070.6	6071.1	6614.3	6622.7
PbH_4	6479.6	6619.3	6493.8	6487.7	5915.3	5938.2	5945.3	6460.9	6492.0
PbO	3590.3	3099.4	3609.3	3563.7	2970.9	2944.3	2944.3	3362.9	3495.2
PbO_2	6826.9	5893.9	6836.1	6839.1	6269.9	6313.2	6313.2	6758.6	6818.2
$PoBr_2$	−7457.3	−6376.2	−7489.4	−7805.4	−8399.3	−7953.0	−7953.0	−7837.1	−7712.5
$PoCl_4$	454.3	793.0	464.5	401.6	−280.9	−53.0	−48.2	355.9	395.2
PoF_2	−12237.8	−11563.0	−12256.7	−12175.9	−12944.2	−12413.2	−12413.2	−12443.0	−12286.0
PoF_6	4365.7	4447.6	4373.1	4304.7	3625.9	3931.7	3931.7	4236.7	4339.4
PoO_2	−1544.2	−3910.6	−1535.0	−1503.6	−2281.0	−2000.9	−2000.9	−1711.2	−1612.7
Rn_2	10093.2	10128.1	10099.7	10108.1	9367.6	9319.5	9319.5	10069.5	10061.5
RnF_2	−1513.3	−2032.8	−1528.4	−732.7	−1674.0	−1299.8	−1299.8	−1018.4	−1080.0
TlCl	7600.9	7888.4	7624.1	7567.7	6983.6	6946.7	6946.2	7500.3	7530.0
$TlCl_3$	6472.2	6528.9	6492.1	6478.6	5922.1	5935.2	5932.0	6430.4	6509.7
TlH	4032.1	4432.6	4090.5	3976.0	3389.0	3426.4	3411.2	3914.4	4007.6
TlH_3	4618.3	4881.7	4656.9	4608.9	4048.3	4087.0	4065.4	4568.0	4680.2

3.2 Double-zeta basis sets

3.2.1 Group 1s

Table 17 NMR isotropic shielding constants of various molecules containing 1s elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
AlH_3	25.5	25.8	25.5	25.4	25.5	25.4	25.5	25.4
AsH_3	28.6	28.6	28.6	28.8	28.5	28.6	28.6	28.5
B_2H_6	31.4	31.6	31.4	31.6	30.7	31.0	31.0	31.5
B_2H_6	26.3	26.6	26.3	26.4	26.4	26.6	26.6	26.4
$B_3N_3H_6$	26.1	26.3	26.1	26.4	27.1	27.0	27.0	26.4
$B_3N_3H_6$	25.1	25.4	25.1	25.3	25.3	25.6	25.6	25.1
B_4H_4	19.9	19.9	19.9	19.9	19.5	19.8	19.8	20.1
BaH_2	23.3	23.5	23.2	23.0	25.5	23.5	23.5	23.5
Be_2H_4	25.8	26.3	25.9	25.9	25.9	25.8	25.8	26.0
Be_2H_4	26.0	26.6	26.4	26.4	24.7	25.4	25.4	26.4
BeC_2H_6	31.7	31.7	31.6	31.9	31.7	31.7	31.7	31.7
$BeF_2O_2H_4$	28.2	28.0	28.2	29.4	28.9	29.3	29.3	28.8
BeH_2	27.4	28.0	28.0	27.8	25.6	26.3	26.3	27.7
BH_3	22.7	23.0	22.7	22.7	22.2	22.5	22.5	22.6
BH_3CO	29.5	29.6	29.5	29.7	29.3	29.6	29.6	29.6
BH_3NH_3	28.8	29.0	28.8	29.0	28.7	29.1	29.1	28.9
BH_3NH_3	28.1	28.3	28.1	28.8	28.0	28.5	28.5	28.4
BiH_3	27.0	27.0	27.0	27.3	27.0	27.1	27.1	27.1
C_2H_2	29.7	29.6	29.7	30.0	27.9	28.5	28.5	29.8
C_2H_3N	30.9	30.9	30.9	31.6	31.4	31.6	31.6	31.2
C_2H_3N	23.7	23.6	23.7	24.2	22.5	22.9	22.9	23.9
C_2H_4	25.2	25.3	25.2	25.6	25.9	26.4	26.4	25.5
C_2H_6	30.0	30.1	30.0	30.3	29.8	30.2	30.2	30.1
C_4H_4	28.0	27.8	28.0	28.6	27.9	28.4	28.4	28.4
C_6H_6	23.4	23.4	23.4	23.9	24.5	24.9	24.9	23.9
CaH_2	26.0	26.0	25.9	25.7	25.7	25.6	25.6	25.6
$Cd(CH_3)_2$	31.1	31.3	31.1	31.4	30.9	31.0	31.0	31.1
CH_2O	20.5	20.9	20.5	21.0	21.6	22.3	22.3	21.2
CH_2O_2	25.9	26.1	25.9	26.0	25.7	26.2	26.2	26.0
CH_3N	20.4	20.3	20.3	21.0	21.2	21.2	21.2	31.2
CH_3N	22.8	22.5	23.0	23.5	24.2	24.2	24.2	23.9
CH_3N	23.1	23.0	23.5	23.9	24.4	24.4	24.4	23.9
CH_4	30.8	30.8	30.8	31.1	30.5	30.8	30.8	30.8
CsH	24.2	24.4	24.1	24.7	24.4	23.9	23.9	23.9
CuH	33.3	31.6	33.3	33.9	34.9	32.5	32.6	32.6
Ferrocene	27.0	27.2	27.0	27.4	27.4	27.9	27.9	27.3
GaH_3	24.2	24.6	24.2	24.3	24.4	24.2	24.2	24.1
GeH_4	27.1	27.2	27.1	27.3	27.2	27.1	27.2	27.1
H_2	26.2	26.2	26.2	26.4	26.0	26.1	26.1	26.0
H_2CO_3	25.8	25.6	25.8	27.0	27.0	27.3	27.3	26.3
H_2O	30.8	30.5	30.8	31.8	31.3	31.6	31.6	31.1
H_2O_2	24.3	24.5	24.3	25.5	24.6	25.1	25.1	24.9
H_2SO_4	26.1	26.0	26.0	27.5	26.4	27.2	27.2	26.8
H_3PO_4	27.5	27.4	27.5	28.8	27.8	28.5	28.5	28.2
HBr	31.1	30.7	31.1	31.4	30.5	31.3	31.3	31.2
$CHBr_3$	22.4	23.0	22.4	23.1	21.5	22.2	22.1	22.8
HCl	30.7	30.4	30.8	31.1	30.3	31.3	31.2	31.1
HCN	28.3	28.3	28.3	28.7	26.2	27.1	27.1	28.7
HCP	28.8	28.9	28.8	28.7	26.0	26.7	26.7	28.8
He_2	59.9	59.8	59.7	59.8	59.7	59.7	59.7	59.7
HF	29.3	28.7	29.3	30.6	29.7	30.0	30.0	29.6
$Hg(CH_3)_2$	30.7	30.9	30.7	31.0	30.9	31.0	31.0	30.7
HI	27.1	27.1	27.0	27.2	24.8	25.5	25.5	27.3
HNC	1.0	1.0	1.0	−0.8	2.4	2.4	2.4	−0.7
HNO	16.3	16.6	16.3	17.2	17.1	18.0	18.0	17.1
HNO_2	21.2	20.9	21.2	22.5	22.1	22.6	22.6	22.0
HNO_3	30.3	30.1	30.3	30.7	30.4	30.8	30.7	30.6
H_2S	27.5	27.6	27.5	28.1	27.1	28.3	28.2	28.1
H_2S_2	31.2	30.8	31.2	31.3	30.3	31.2	31.2	31.2
InH	21.8	22.1	21.8	21.6	19.9	21.1	21.2	21.1

InH_3	21.8	24.7	24.3	24.3	24.5	24.3	24.3	24.2
KH	24.9	25.2	24.9	25.1	24.8	24.7	24.7	24.7
LaH_3	21.9	22.3	21.9	21.6	21.5	21.4	21.4	21.4
$Li_4C_4H_{12}$	32.6	32.7	32.6	32.8	32.4	32.6	32.6	32.6
Li_4H_4	27.7	27.8	27.7	27.6	27.9	27.5	27.5	27.6
$LiBH_4$	30.2	30.3	30.2	30.4	30.1	30.0	30.0	30.2
$LiBH_4$	31.3	31.4	31.4	31.4	31.0	31.1	31.1	31.3
LiH	26.1	26.3	26.2	26.0	25.7	25.8	25.8	25.8
MgH_2	26.5	26.7	26.5	26.3	26.2	26.1	26.3	26.2
H_2N_2	14.3	14.7	14.3	14.5	15.7	16.0	16.0	14.4
N_2H_4	28.3	28.0	29.1	28.2	28.7	28.7	28.7	28.8
N_2H_4	28.4	28.2	29.2	28.6	29.0	29.0	29.0	28.8
NaH	25.6	25.8	25.6	25.5	25.2	25.4	25.4	25.4
NH_3	31.3	31.2	31.3	32.0	31.3	31.6	31.6	31.5
NH_3HF	30.3	30.2	30.3	30.8	30.1	30.5	30.5	30.4
NH_3HF	22.0	21.3	21.9	23.5	22.0	22.9	22.9	22.1
PbH_4	26.4	26.5	26.4	26.6	26.5	26.5	26.5	26.5
PH_3	29.1	29.0	29.1	29.4	29.1	29.3	29.2	29.1
RbH	24.6	24.9	24.6	24.8	24.6	24.2	24.2	24.2
SbH_3	27.5	27.6	27.6	27.8	27.5	27.7	27.7	27.7
ScH_3	24.0	24.8	24.0	23.8	25.2	24.4	24.5	24.2
SeH_2	29.9	29.8	30.0	30.2	29.9	30.2	30.2	30.1
SiH_4	27.4	27.5	27.4	27.7	27.3	27.5	27.6	27.5
SnH_4	26.6	26.7	26.6	26.7	26.6	26.7	26.7	26.6
SrH_2	24.5	24.8	24.5	24.4	25.8	24.2	24.2	24.2
TeH_2	29.2	29.0	29.2	29.4	29.3	29.5	29.5	29.5
TiH_4	19.4	19.8	19.4	19.2	18.0	18.6	18.7	18.6
TlH	21.5	21.7	21.5	21.4	19.5	21.2	21.3	21.2
TlH_3	23.6	24.0	23.6	23.8	24.1	23.8	23.8	23.8
VH_5	10.8	7.7	10.8	10.6	10.7	9.3	9.6	9.6
VH_5	15.2	14.9	15.2	15.2	12.9	14.5	14.6	14.6
ZnH_2	26.7	26.9	26.7	26.7	25.9	26.3	26.3	26.3
$Zn(CH_3)_2$	31.2	31.3	31.1	31.4	30.9	31.1	31.1	31.2

3.2.2 Group 2s

Table 18 NMR isotropic shielding constants of various molecules containing 2s elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Be_2F_4	103.6	105.1	101.9	106.0	112.5	112.6	112.6	105.7
Be_2H_4	79.7	82.5	78.3	82.5	86.1	91.5	91.5	82.3
Be_4	139.5	137.9	138.7	140.2	144.5	140.5	140.5	136.7
BeC_2H_6	70.6	72.6	69.2	74.3	75.9	82.1	82.1	72.9
$BeF_2O_2H_4$	104.6	106.2	103.1	107.4	113.2	112.8	112.8	107.8
BeH_2	75.4	77.3	73.8	78.2	80.5	86.7	86.7	77.9
BeS	97.4	98.4	96.0	98.7	109.6	103.9	103.9	91.2
Li_2	98.6	98.2	98.4	98.7	99.8	98.5	98.5	98.2
Li_2O	84.3	85.3	83.8	85.4	87.5	83.8	83.8	83.3
$Li_4C_4H_{12}$	85.0	85.8	84.4	85.4	87.5	83.8	83.8	84.9
Li_4Cl_4	88.6	89.2	88.1	89.6	92.9	89.9	89.9	89.3
Li_4H_4	87.2	87.6	86.7	87.9	91.7	87.2	87.2	86.9
Li_8	101.3	101.3	100.9	101.5	104.0	101.0	101.0	100.6
$LiBH_4$	90.3	90.9	89.9	91.0	93.7	90.6	90.6	90.2
LiCl	87.6	88.0	86.9	88.4	92.8	87.0	87.1	86.7
LiF	87.3	87.9	86.5	88.2	91.4	86.1	86.1	86.1
LiH	89.2	88.7	88.6	89.5	93.2	89.7	89.7	89.0
Li_2S	86.2	86.5	85.4	86.8	91.4	85.4	85.5	84.7
Li_3P	89.7	89.2	89.0	90.3	94.8	90.1	90.0	89.1

3.2.3 Group 2p

Table 19 NMR isotropic shielding constants of various molecules containing 2p elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Al_2O_3	291.2	299.0	291.4	302.2	292.9	306.5	307.7	311.9
Al_2O_3	217.8	229.7	218.1	191.9	205.2	208.7	210.0	193.1
AlF_3	378.4	390.3	378.7	356.1	349.3	365.2	365.3	412.3
AtF_3	174.1	228.6	175.1	163.0	142.5	167.1	167.3	188.9
AtF_3	205.2	256.4	206.3	200.8	180.5	203.3	203.5	226.6
B_2H_6	72.2	79.3	72.5	80.8	81.6	88.1	88.1	74.7
$B_3N_3H_6$ (B)	65.7	69.6	65.9	76.4	76.5	82.0	82.0	69.5
$B_3N_3H_6$ (N)	103.2	115.9	103.7	116.9	119.1	127.3	127.3	108.9
B_4H_4	−81.6	−83.1	−80.9	−65.1	−61.5	−52.0	−52.0	−75.6
BaF_2	−18.1	45.9	−8.5	−84.5	197.9	−35.8	−34.3	−17.0
BaO	−705.6	−844.6	−768.6	−794.8	608.8	−607.1	−606.0	−701.2
Be_2F_4	347.4	360.0	347.4	354.8	370.6	355.8	355.8	386.5
Be_2F_4	355.5	367.5	355.5	352.4	316.9	346.3	346.3	365.1
BeC_2H_6	192.6	195.9	192.8	197.7	196.3	198.8	198.8	192.2
$BeF_2O_2H_4$ (F)	368.7	379.9	368.8	353.7	360.7	358.1	358.1	393.0
$BeF_2O_2H_4$ (O)	283.0	289.5	283.2	297.9	296.6	295.2	295.2	291.7
BF_3 (B)	82.2	88.0	82.4	93.1	93.4	97.6	97.6	85.8
BF_3 (F)	289.0	303.4	289.3	285.6	290.7	300.8	300.8	308.3
BH_3	−7.8	2.2	−7.3	4.6	7.8	17.5	17.5	−4.5
BH_3CO (B)	157.1	158.9	157.2	161.3	160.4	164.7	164.7	158.5
BH_3CO (C)	−18.6	−19.5	−17.8	1.8	3.2	12.7	12.7	−11.8
BH_3CO (O)	−47.4	−49.6	−46.6	−29.7	−21.5	−8.1	−8.1	−47.4
BH_3NH_3 (B)	116.9	121.6	117.1	123.9	124.5	130.8	130.8	119.7
BH_3NH_3 (N)	216.2	223.2	216.4	223.7	221.8	226.4	226.4	216.7
BiF_3	152.7	198.0	153.6	142.3	133.0	147.5	147.6	187.6
C_2H_2	104.5	106.5	105.0	115.7	117.5	122.6	122.6	106.3
C_2H_3N (N)	225.4	235.2	225.7	228.2	229.2	229.0	229.0	223.6
C_2H_3N (C)	53.5	57.8	54.0	67.1	68.2	74.8	74.8	56.8
C_2H_4	43.4	47.0	44.0	58.0	59.8	67.8	67.8	47.2
C_2H_6	167.4	172.4	167.7	174.1	173.4	178.9	178.9	168.4
C_4H_4	204.0	209.1	204.2	207.9	207.7	208.4	208.4	203.9
C_6H_6	40.0	43.1	40.6	55.4	56.7	65.3	65.3	46.6
CaF_2	159.9	249.2	209.2	253.1	353.2	140.9	143.5	245.2
CdF_2	400.6	449.2	401.6	353.1	369.1	367.4	367.3	422.9
$Cd(CH_3)_2$	185.2	193.0	185.4	190.1	191.8	191.6	191.6	184.5
CF_4 (C)	35.1	46.3	35.7	53.6	52.7	58.4	58.4	43.1
CF_4 (F)	216.9	232.9	217.5	235.6	236.2	246.1	246.1	238.3
CH_2O (C)	−29.4	−23.9	−28.7	−5.9	−5.9	2.6	2.6	−18.8
CH_2O (O)	−448.6	−453.7	−446.7	−435.0	−420.1	−405.0	−405.0	−476.5
CH_2O_2 (C)	83.4	90.1	83.9	95.9	95.4	100.7	100.7	87.1
CH_2O_2 (O)	21.6	40.9	22.5	34.1	39.6	45.6	45.6	17.4
CH_3N (N)	−132.2	−131.3	−131.0	−116.0	−107.3	−98.0	−98.0	−138.6
CH_3N (C)	1.0	4.7	1.6	21.3	22.3	31.2	31.2	8.9
CH_4	185.0	187.8	185.2	190.3	189.7	193.0	193.0	183.5
ClF	629.7	639.6	628.6	582.4	607.8	560.7	560.9	600.5
ClF_3	−182.6	−98.0	−180.2	−162.1	−178.2	−160.0	−162.1	−173.8
ClF_3	21.7	29.9	21.9	31.0	51.5	27.8	27.0	24.4
CO (C)	−21.9	−25.6	−21.1	−6.1	−3.1	7.7	7.7	−16.8
CO (O)	−95.8	−100.0	−94.8	−78.6	−71.4	−54.5	−54.5	−96.5
CO_2 (C)	47.5	47.1	48.1	65.1	65.6	72.2	72.2	52.3
CO_2 (O)	199.0	200.3	199.4	205.5	211.7	217.4	217.4	199.6
$Cr(CO)_6$ (C)	−42.7	−53.0	−41.9	−20.3	−18.5	−11.1	−10.9	−34.8
$Cr(CO)_6$ (O)	−103.0	−114.5	−102.0	−85.1	−76.9	−56.6	−56.2	−99.9
CrO_3	−1446.0	−1868.7	−1440.3	−1358.8	−1363.8	−1363.1	−1348.0	−1495.3
CS_2	−24.5	−36.6	−23.8	−4.2	−2.9	4.0	3.8	−13.5
CsF	119.2	179.5	113.7	352.1	320.0	46.9	48.6	71.2
Cu_2O	582.3	616.2	581.2	579.3	630.8	546.7	552.8	577.2
CuCN (C)	68.7	55.9	69.3	87.4	89.9	91.2	91.5	76.5
CuCN (N)	−119.3	−119.0	−118.2	−106.6	−99.6	−83.7	−84.1	−122.8
CuF	677.1	637.0	675.1	660.7	746.1	648.0	655.5	711.5
F_2	−274.9	−246.5	−273.1	−240.1	−232.3	−219.3	−219.3	−289.8

$Fe(CO)_5$ (C)	−45.6	−53.6	−44.8	−23.1	−21.6	−12.2	−12.2	−37.3
$Fe(CO)_5$ (C)	−60.4	−73.4	−59.5	−36.5	−37.8	−30.3	−30.2	−51.4
$Fe(CO)_5$ (O)	−103.6	−106.5	−102.6	−86.7	−73.9	−54.3	−54.2	−98.2
$Fe(CO)_5$ (O)	−137.2	−160.6	−136.2	−120.4	−109.9	−90.1	−89.6	−131.7
Ferrocene	99.8	107.5	100.3	111.6	112.6	117.3	117.4	103.2
GaF	72.4	118.9	73.9	19.9	26.7	30.9	30.6	82.5
GeF_4	298.0	328.2	298.5	279.1	273.4	289.3	289.3	315.0
GeO	−424.7	−430.9	−422.5	−435.8	−417.4	−401.7	−401.6	−465.7
GeO_2	−51.4	−59.5	−50.2	−61.5	−48.4	−36.6	−35.8	−71.6
H_2CO_3 (C)	13.6	16.4	14.2	33.6	35.9	42.3	42.4	22.3
H_2CO_3 (O)	12.2	13.4	12.8	28.5	37.9	48.5	48.5	13.4
H_2CO_3 (O)	147.1	155.9	147.4	167.1	170.1	177.6	177.6	158.4
H_2O	318.4	319.9	319.0	334.0	330.9	333.4	333.4	330.0
H_2O_2	84.1	98.9	84.8	93.0	96.7	106.8	106.8	82.5
H_2SO_4 (O)	19.5	36.1	20.3	35.4	37.8	50.4	50.0	24.7
H_2SO_4 (O)	81.5	93.6	82.3	106.6	97.2	114.5	114.7	99.5
H_3PO_4	193.6	204.8	194.2	214.5	203.2	219.3	219.3	209.7
$H_3\ PO_4$	150.1	163.8	150.7	156.3	156.7	172.0	171.4	151.4
$CHBr_3$	54.5	70.1	54.9	67.0	66.3	75.6	75.6	59.4
HCN (C)	67.1	66.6	67.7	82.0	83.0	90.1	90.1	70.9
HCN (N)	−52.8	−55.4	−51.9	−36.9	−28.7	−19.9	−19.9	−55.7
HCP	10.3	9.6	11.0	26.0	28.0	35.6	35.4	14.6
HF	403.4	405.4	403.6	407.1	407.1	411.7	411.7	434.1
HfO	−724.8	−780.6	−722.4	−692.9	−684.8	−655.8	−655.6	−749.3
HfO_2	−455.8	−522.3	−453.9	−435.4	−415.6	−413.6	−412.8	−497.5
HgF_2	359.4	423.9	360.0	312.3	351.5	321.1	321.6	367.4
$Hg(CH_3)_2$	175.3	183.5	175.5	181.1	187.1	181.8	181.8	174.5
HNC (N)	85.6	84.4	86.2	102.8	103.8	109.3	109.3	88.5
HNC (C)	1.3	−1.2	2.0	16.3	19.5	27.9	27.9	3.5
HNO (O)	−2126.4	−2294.5	−2119.3	−2113.6	−2095.8	−2120.7	−2120.8	−2314.9
HNO (N)	−1052.9	−1128.0	−1048.4	−1012.8	−995.7	−1005.0	−1005.0	−1117.0
HNO_2 (N)	−121.2	−146.4	−120.3	−86.3	−84.1	−75.6	−75.6	−103.8
HNO_2 (O)	−375.0	−392.8	−373.2	−348.4	−338.4	−320.3	−320.3	−380.3
HNO_3 (N)	−98.9	−116.7	−98.0	−67.7	−66.6	−60.1	−60.1	−82.2
HNO_3 (O)	−199.5	−217.7	−198.5	−167.1	−159.5	−141.9	−141.9	−186.4
HNO_3 (O)	−101.0	−99.9	−100.1	−78.2	−71.2	−55.5	−55.5	−91.6
HNO_3 (O)	−194.3	−222.5	−193.1	−158.8	−149.5	−138.0	−138.0	−184.5
KF	296.2	313.6	284.9	376.0	360.4	262.3	262.7	377.3
LaF_3	−78.6	−17.6	−68.4	−66.8	−200.8	−113.9	−112.1	−85.6
Li_2O	159.9	165.9	159.7	175.4	232.6	179.3	179.3	180.4
$Li_4C_4H_{12}$	193.6	197.8	193.8	199.6	198.5	199.9	199.9	192.9
$LiBH_4$	142.4	145.0	142.5	147.3	149.1	150.4	150.4	142.9
LiF	341.9	361.3	342.6	291.0	284.2	261.3	261.3	366.5
MgF_2	427.9	434.6	428.0	388.1	407.0	400.5	401.2	449.1
$Mo(CO)_6$ (C)	−36.3	−43.2	−35.5	−13.6	−13.3	−5.2	−5.1	−27.9
$Mo(CO)_6$ (O)	−99.3	−107.4	−98.3	−81.1	−72.3	−53.2	−53.1	−96.6
MoO_3	−736.1	−880.2	−733.0	−705.5	−682.2	−680.1	−677.9	−769.9
N_2	−98.6	−106.8	−97.4	−83.1	−75.9	−59.9	−59.9	−94.4
N_2H_2	−380.2	−386.6	−378.6	−339.9	−328.4	−326.3	−326.3	−387.8
N_2H_4	185.4	193.6	185.8	192.3	192.2	198.5	198.5	186.2
N_4	206.2	213.1	206.6	211.6	214.4	212.8	212.8	207.0
Na_2O	326.4	385.3	329.5	324.3	417.6	335.8	335.8	355.5
Na_3N	−135.6	−340.3	−130.7	−146.6	−92.4	−94.4	−95.4	−129.8
NaF	445.8	455.9	447.6	379.7	381.1	376.9	375.3	475.1
NbO_2F (O)	−761.1	−866.1	−758.0	−731.4	−707.8	−693.9	−691.5	−787.3
NbO_2F (F)	53.9	102.3	55.0	25.8	39.0	41.8	42.4	67.8
Ne_2	550.1	550.7	550.0	552.7	551.4	551.6	551.6	552.5
NF_3 (N)	−197.8	−179.5	−196.5	−168.3	−165.0	−154.1	−154.1	−190.7
NF_3 (F)	−30.7	3.2	−29.9	17.9	18.6	30.7	30.7	0.9
NH_3	254.8	256.3	255.0	265.7	262.4	263.6	263.6	259.1
NH_4F (N)	242.3	245.3	242.5	250.3	246.5	248.8	248.8	244.2
NH_4F (F)	365.1	370.8	364.8	400.2	400.8	407.4	407.4	445.4
$Ni(CO)_4$ (C)	−29.3	−33.8	−28.5	−7.9	−7.9	0.8	0.8	−21.8
$Ni(CO)_4$ (O)	−90.7	−97.4	−89.8	−73.5	−59.7	−43.6	−43.4	−85.4
OF_2 (O)	−700.7	−624.7	−698.6	−626.1	−612.8	−577.9	−578.0	−679.4
OF_2 (F)	−122.8	−85.6	−121.6	−86.9	−80.3	−70.8	−70.8	−116.8
$Os(CO)_5$ (C)	−48.9	−50.6	−48.1	−26.1	−24.0	−17.7	−17.7	−77.4

$Os(CO)_5$ (C)	−51.1	−53.6	−50.2	−27.6	−30.4	−20.4	−20.3	−42.8
$Os(CO)_5$ (O)	−131.3	−119.2	−119.2	−110.9	−94.4	−84.2	−84.1	−127.8
$Os(CO)_5$ (O)	−124.0	−130.0	−123.1	−104.7	−94.8	−78.8	−78.7	−120.8
OsO_3	−766.4	−739.5	−739.5	−729.6	−716.2	−721.3	−719.0	−805.4
OsO_4	−553.7	−699.1	−552.4	−529.9	−505.5	−538.1	−535.8	−612.9
PbO	−679.2	−726.8	−676.7	−723.5	−697.0	−682.7	−682.5	−766.4
PbO_2	−512.7	−603.2	−511.0	−551.3	−530.2	−502.8	−502.7	−565.6
$Pd(CO)_4$ (C)	−27.2	−29.5	−26.5	−6.5	−6.8	1.8	1.8	−19.8
$Pd(CO)_4$ (O)	−100.6	−104.3	−99.6	−82.7	−69.9	−56.3	−56.3	−98.8
PF_3	159.0	169.1	169.1	178.0	157.4	185.5	184.8	204.8
PF_5	184.4	204.6	185.2	198.1	181.4	208.6	208.7	205.0
PF_5	194.6	215.3	195.6	202.0	187.3	215.4	215.2	219.9
PoF_2	364.0	426.4	364.8	359.4	339.5	359.5	359.6	404.8
PoF_6	−377.2	−220.4	−374.5	−414.2	−419.7	−375.6	−374.8	−394.0
PoO_2	−1261.5	−1553.8	−1256.8	−1311.3	−1251.2	−1265.8	−1264.8	−1384.3
$Pt(CO)_4$ (C)	−27.7	−30.7	−26.9	−6.5	−5.3	1.9	1.9	−19.9
$Pt(CO)_4$ (O)	−97.1	−101.1	−96.2	−79.0	−63.6	−57.5	−57.3	−99.0
PtO_2	−256.1	−246.0	−255.3	−237.0	−224.0	−224.4	−223.5	−267.8
RbF	243.6	287.5	256.3	352.4	352.8	148.8	153.4	207.8
Re_2O_7	−10.2	20.9	−9.7	11.8	−1.7	−4.6	−3.4	−19.6
Re_2O_7	−549.8	−657.4	−548.3	−524.8	−507.2	−520.1	−518.4	−594.9
RnF_2	142.9	206.3	144.9	4.0	44.4	5.9	7.2	87.1
$Ru(CO)_5$ (C)	−48.7	−51.4	−47.8	−25.8	−21.7	−15.7	−15.7	−39.5
$Ru(CO)_5$ (C)	−55.1	−59.4	−54.2	−31.4	−34.4	−25.4	−25.3	−46.2
$Ru(CO)_5$ (O)	−130.9	−131.5	−129.8	−111.2	−98.7	−80.4	−80.4	−127.2
$Ru(CO)_5$ (O)	−135.4	−144.3	−134.3	−115.8	−109.5	−89.2	−89.1	−132.4
RuO_2	−475.8	−581.5	−474.0	−446.3	−432.9	−416.9	−415.9	−479.5
RuO_4	−789.8	−1077.1	−787.0	−757.3	−736.9	−742.5	−740.0	−829.3
SbF_3	165.8	206.9	167.1	154.4	145.2	162.2	162.7	200.5
ScF_3	−67.5	−0.6	−66.0	−76.3	−69.6	−78.5	−67.1	−63.0
SeO_2	−673.1	−751.3	−670.7	−662.8	−627.5	−624.1	−624.6	−701.6
SF_2	292.7	328.4	293.2	320.2	300.1	319.5	319.1	332.7
SF_4	−9.6	23.2	−8.1	32.0	4.0	37.9	36.9	37.8
SF_4	35.6	72.6	36.7	68.1	54.2	75.8	75.0	75.0
SF_6	6.7	38.0	7.7	30.3	16.8	47.4	47.8	34.9
SiF_4	324.4	338.3	325.1	319.2	303.4	329.3	328.9	355.4
SiO_2	172.2	180.4	172.3	139.2	165.5	161.5	162.8	141.8
SnO	−623.0	−649.9	−618.0	−654.4	−625.0	−615.5	−615.1	−695.2
SnO_2	−310.2	−360.2	−307.2	−337.1	−304.0	−303.4	−301.4	−354.3
SrF_2	111.6	154.7	113.4	36.1	310.5	57.4	61.8	103.2
SrO	−402.5	−522.7	−400.5	−357.4	79.6	−354.2	−346.5	−439.3
TaF_3	−80.0	−22.1	−78.4	−95.9	−91.6	−77.3	−77.0	−76.1
TaO_2F (F)	78.7	112.8	79.8	49.4	61.6	54.1	54.7	84.9
TaO_2F (O)	−726.6	−756.0	−723.8	−712.7	−710.5	−697.6	−695.9	−794.6
Tc_2O_7	−124.3	−84.6	−123.3	−99.0	−106.1	−103.3	−102.8	−119.3
Tc_2O_7	−750.5	−947.3	−747.8	−717.7	−694.5	−693.8	−692.6	−779.7
TcO_3F (F)	88.3	149.4	89.0	64.7	78.4	79.7	79.9	92.0
TcO_3F (O)	−746.9	−949.5	−744.0	−713.0	−690.6	−691.7	−690.3	−779.0
TeO_2	−896.8	−1029.1	−893.2	−914.2	−862.8	−889.9	−889.1	−984.3
$Ti(CO)_4$ (C)	−428.2	−630.9	−426.0	−381.2	−385.1	−364.9	−365.3	−399.5
$Ti(CO)_4$ (O)	−1225.2	−1973.1	−1221.1	−1183.7	−1168.2	−1097.7	−1099.8	−1227.8
TiF_4	−179.6	−147.6	−177.9	−178.5	−169.5	−183.4	−174.5	−191.5
TiO_2	−829.5	−964.3	−826.6	−775.3	−770.8	−749.6	−742.6	−851.3
$W(CO)_6$ (C)	−32.8	−38.4	−32.0	−10.4	−10.6	−0.5	−0.5	−24.3
$W(CO)_6$ (O)	−90.9	−97.3	−90.0	−71.5	−60.5	−46.2	−46.2	−88.9
WO_3	−943.9	−969.9	−940.6	−938.1	−940.3	−959.6	−955.6	−1066.5
XeF_2	256.3	301.0	256.7	200.4	194.0	181.9	183.3	219.6
XeF_4	42.9	89.8	43.9	45.6	21.8	39.2	40.4	44.7
$XeOF_4$ (O)	−398.3	−407.5	−397.8	−401.7	−393.3	−391.8	−390.3	−449.9
$XeOF_4$ (F)	−139.5	−76.9	−137.4	−127.1	−151.1	−123.1	−122.0	−132.2
YF	−200.0	−131.9	−197.6	−230.0	−205.1	−199.5	−198.9	−228.6
YF_3	25.6	74.6	27.0	−16.9	7.0	9.3	9.5	−44.7
ZnF_2	412.4	443.2	412.8	375.8	391.5	402.0	402.1	444.1
$Zn(CH_3)_2$	184.4	191.6	184.7	189.6	192.1	195.0	194.9	187.5
ZrO	−778.4	−892.1	−775.4	−746.3	−719.1	−692.8	−691.1	−784.2
ZrO_2	−734.5	−806.1	−731.6	−721.2	−685.1	−667.1	−666.0	−765.9

3.2.4 Group 3s

Table 20 NMR isotropic shielding constants of various molecules containing 3s elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Mg_4	707.2	710.1	707.2	707.5	705.9	705.3	704.4	706.1
$MgCl_2$	496.9	507.1	497.2	502.0	508.4	505.8	491.7	493.9
MgF_2	538.2	550.0	538.4	538.3	535.1	550.7	533.8	534.3
MgH_2	426.1	437.3	426.5	433.0	432.5	449.9	420.8	422.8
Na_2	610.7	608.3	610.6	611.5	610.1	622.6	610.5	612.3
Na_2O	584.7	574.0	584.4	586.1	576.7	605.8	579.9	584.0
Na_2S	567.6	562.6	567.5	567.8	565.1	597.4	565.3	570.9
Na_3N	588.6	582.1	588.3	591.4	588.3	615.8	584.9	590.2
Na_3P	581.9	573.1	581.7	584.4	582.7	616.4	579.4	586.4
Na_3P	582.0	573.2	581.8	584.5	582.9	616.4	579.6	586.5
Na_3P	582.5	573.7	582.3	585.0	583.3	616.5	580.1	587.0
NaCl	570.1	569.9	570.1	572.2	568.3	602.4	574.6	579.7
NaF	580.1	580.3	580.0	583.5	579.1	612.7	585.8	587.4
NaH	577.3	572.4	577.2	579.2	573.8	594.0	576.8	579.3

3.2.5 Group 3p

Table 21 NMR isotropic shielding constants of various molecules containing 3p elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
AgCl	960.7	1087.1	961.1	920.0	948.3	961.9	946.9	955.7
Al_2O_3	478.6	477.6	479.0	492.3	509.8	519.3	483.2	469.8
Al_2S_3 (Al)	379.3	377.3	379.9	394.9	410.0	418.8	383.1	371.0
Al_2S_3 (S)	647.5	693.0	648.5	644.9	675.1	701.3	649.4	680.6
Al_2S_3 (S)	590.5	633.9	591.3	557.5	603.5	606.3	551.0	583.3
$AlCl_3$ (Al)	398.0	413.2	398.4	408.1	428.1	430.5	396.2	384.5
$AlCl_3$ (Cl)	877.4	912.2	878.2	863.9	875.1	890.2	868.8	881.8
AlF_3	492.9	509.0	492.9	494.5	526.3	517.2	490.3	484.5
AlH_3	254.7	281.7	255.6	266.4	280.8	289.8	252.4	241.3
Ar_2	1240.6	1241.0	1240.5	1242.4	1230.8	1239.6	1242.7	1242.4
As_4S_4	721.6	772.2	722.6	753.6	732.0	779.6	753.1	769.2
$AsCl_3$	480.0	551.3	480.5	483.4	473.1	536.6	476.9	511.7
AtCl	1214.8	1268.5	1215.3	1247.8	1235.0	1215.9	1250.8	1227.3
AuCl	812.1	995.7	812.7	804.4	834.9	779.3	745.5	763.5
BaS	−236.3	−397.3	−303.7	−232.2	911.9	2.1	−123.7	−136.1
BeS	1073.2	1038.3	1074.1	1081.5	1073.3	1066.5	1057.7	1080.1
BrCl	692.0	742.2	692.1	696.4	679.3	705.1	675.6	689.7
$CaCl_2$	794.2	904.4	863.7	963.0	1032.0	817.4	785.4	805.3
Cd_2Cl_2	817.2	894.0	817.8	785.8	817.6	802.5	773.0	789.9
Cl_2	417.8	462.4	419.5	405.1	404.6	442.2	375.0	414.9
ClF	−846.1	−782.6	−839.2	−623.5	−713.3	−517.8	−695.6	−672.0
ClF_3	−955.9	−752.8	−948.3	−823.3	−903.0	−703.4	−892.9	−825.5
CS_2	472.0	479.5	473.4	478.2	468.9	538.3	475.4	513.5
Cu_2S	920.8	984.1	921.4	949.1	949.2	955.9	961.7	959.0
CuCl	1123.3	1161.0	1123.9	1125.3	1160.2	1141.8	1157.0	1150.8
GaCl	436.0	498.7	437.9	405.0	423.7	417.4	347.7	386.0
$GaCl_3$	740.8	815.7	742.0	726.5	732.7	755.2	716.9	739.0
$GeCl_4$	565.9	652.6	567.3	555.2	549.2	605.8	550.5	582.9
H_2SO_4	117.8	120.5	122.7	160.5	133.6	213.0	133.4	177.1
H_3PO_4	260.7	279.3	263.1	286.7	271.0	352.0	261.0	256.9
HCl	926.5	934.9	928.0	926.1	913.8	945.5	921.2	936.9
HCP	323.2	321.4	324.1	324.2	328.7	373.1	296.9	292.0
Hg_2Cl_2	695.4	801.9	696.2	662.1	722.8	660.6	596.4	634.1
H_2S	690.7	699.4	693.0	693.2	678.9	724.4	675.1	704.5
H_2S_2	525.7	552.3	527.9	531.9	522.7	570.2	510.7	545.2
ICl	1109.7	1151.3	1107.8	1121.8	1107.4	1093.9	1112.9	1100.1
InCl	493.1	570.0	496.7	448.2	467.1	450.4	385.7	421.3
$InCl_3$	810.6	893.7	812.2	778.3	786.2	796.8	765.9	784.5
K_2S	744.7	837.0	735.1	718.3	712.2	858.7	852.1	854.3
K_3P	386.0	377.2	397.2	253.7	309.5	450.9	391.2	383.7
KCl	1006.6	1013.9	990.8	1100.7	1071.7	1036.4	1025.9	1033.2
$LaCl_3$	352.8	435.6	360.3	327.9	226.4	319.0	237.8	282.9
Li_4Cl_4	995.2	1015.7	995.1	1000.6	993.8	1042.7	1038.3	1040.7
LiCl	1017.9	1032.5	1018.0	973.6	1016.7	988.2	974.4	982.1
Li_2S	864.5	869.3	863.6	871.5	924.7	968.8	944.5	958.3
$MgCl_2$	1062.7	1078.8	1062.9	1040.8	1040.4	1039.3	1032.2	1037.2
Na_2S	1031.3	1058.5	1032.1	1037.0	1082.3	1071.2	1082.8	1076.7
Na_3P	561.0	582.1	564.3	538.0	574.7	599.9	557.0	553.4
NaCl	1116.0	1128.9	1116.9	1069.5	1095.1	1080.8	1073.5	1077.3
P_2	−337.5	−373.3	−335.2	−338.9	−303.3	−232.4	−370.8	−380.5
PF_3	135.8	165.2	137.9	145.1	139.4	215.9	120.4	116.7
PF_5	324.0	353.6	326.0	336.7	329.0	394.6	314.1	311.8
PH_3	567.8	577.1	569.1	581.9	569.7	615.6	556.0	553.7
Li_3P	520.1	500.8	519.3	523.5	566.6	689.3	648.0	643.4
$PoCl_4$	467.6	550.8	469.2	438.6	445.0	482.5	428.8	458.9
$PoCl_4$	469.4	551.8	471.0	439.1	447.1	480.4	426.7	456.7
S_5	5.8	43.9	8.4	18.6	10.6	−24.7	−13.9	44.8
S_5	−86.3	−64.4	−84.0	−95.7	−90.6	89.1	−135.6	−73.1
S_5	−181.5	−184.9	−179.1	−175.5	−173.5	−87.4	−210.7	−140.4
$ScCl_3$	314.5	416.7	316.1	296.2	304.2	299.5	229.5	269.8
SF_2	−1172.5	−1093.0	−1163.5	−1017.5	−1138.5	−843.6	−1068.9	−979.7

SF_4	−105.7	−54.4	−101.4	−91.1	−107.9	−25.4	−129.3	−63.2
SF_6	206.7	250.3	210.8	236.5	206.1	260.5	208.8	243.6
$SiCl_4$ (Si)	311.9	330.2	313.5	325.5	331.1	359.4	302.9	298.5
$SiCl_4$ (Cl)	684.5	732.1	686.0	696.5	681.6	735.5	693.2	718.5
SiF_4	429.8	451.2	431.2	436.6	454.8	493.7	420.4	421.4
SiH_4	432.7	445.0	434.1	458.7	440.7	491.7	436.1	432.3
SiO_2	326.0	323.1	327.3	345.4	359.7	403.5	323.1	317.6
SiS_2 (Si)	192.6	180.5	194.0	212.2	228.6	258.2	187.9	182.2
SiS_2 (S)	565.7	594.6	565.9	527.1	576.5	583.1	524.0	558.8
SrS	361.3	303.4	363.4	408.4	307.4	397.5	312.5	360.4
$TiCl_4$	39.9	56.7	42.3	31.7	34.6	30.1	−72.4	−10.6
TiS_2	−891.9	−1124.0	−888.2	−879.2	−883.5	−789.6	−987.3	−872.1
TlCl	471.8	564.6	474.9	426.3	441.6	426.6	363.6	397.1
$TlCl_3$	550.5	694.0	551.9	505.0	506.3	549.2	494.1	525.1
$ZnCl_2$	947.4	1005.0	947.9	929.7	945.8	972.8	968.0	971.5

3.2.6 Group 4s

Table 22 NMR isotropic shielding constants of various molecules containing 4s elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Ca_4	1309.1	1423.1	1399.6	1431.3	1426.8	1387.0	1368.1	1364.1
$CaCl_2$	989.9	1104.9	1065.2	1113.7	1097.4	1064.6	1052.5	1050.8
CaF_2	1100.8	1194.6	1158.2	1188.4	1146.2	1169.2	1146.9	1146.7
CaH_2	824.9	922.7	890.4	937.1	932.6	870.7	843.4	839.6
K_2	1292.8	1284.0	1291.3	1293.8	1292.6	1307.9	1292.9	1290.9
K_2S	1262.9	1241.1	1252.2	1256.3	1257.5	1304.5	1273.6	1280.3
K_3P	1265.5	1240.0	1257.6	1263.8	1262.2	1302.3	1271.5	1271.8
KBr	1253.2	1248.8	1245.2	1243.8	1241.8	1280.9	1265.5	1274.8
KCl	1257.9	1253.9	1249.9	1247.7	1246.0	1291.6	1274.2	1285.6
KF	1289.0	1282.7	1278.8	1281.8	1276.5	1326.8	1313.1	1311.6
KH	1247.3	1230.8	1240.4	1238.2	1233.3	1249.3	1243.9	1245.5
KI	1249.3	1244.8	1242.2	1242.4	1240.6	1272.2	1260.0	1268.8

3.2.7 Group 3d

Table 23 NMR isotropic shielding constants of various molecules containing 3d elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
$Cr(CO)_6$	−547.2	−904.3	−545.8	−517.5	−471.9	−313.9	−413.7	−495.2
CrO_3	−3477.8	−4780.2	−3474.2	−3444.7	−3254.0	−3049.3	−3090.6	−3220.2
Cu_2	2130.3	2240.1	2132.2	2158.1	2084.3	2193.7	2189.5	2182.7
Cu_2O	−753.0	35.7	−743.4	−769.1	−964.7	−127.6	−195.9	−230.0
Cu_2S	518.8	1119.5	525.1	498.3	409.0	875.3	822.4	790.4
CuCl	1141.0	1468.2	1147.7	1079.5	1003.4	1370.5	1345.6	1320.3
CuCN	1222.8	1469.2	1224.2	1191.9	1138.9	1449.6	1400.5	1390.3
CuF	−37.0	603.6	−17.4	−213.9	−440.4	453.3	401.4	363.1
CuH	1444.0	1656.5	1448.5	1389.3	1307.2	1654.7	1621.8	1607.9
$Fe(CO)_5$	−1859.1	−2854.2	−1856.8	−1821.5	−1722.6	−1542.4	−1599.9	−1688.4
Ferrocene	−2485.8	−4718.8	−2483.5	−2475.4	−2437.1	−2241.2	−2254.1	−2346.8
$Ni(CO)_4$	−1636.6	−2029.4	−1634.5	−1566.0	−1395.3	−1211.7	−1312.3	−1393.8
$ScCl_3$	175.2	357.4	176.2	174.8	211.0	265.5	234.1	231.0
ScF_3	633.9	759.6	634.8	629.9	654.2	731.4	675.2	665.2
ScH_3	−450.2	−268.3	−448.9	−445.9	−379.2	−349.5	−402.5	−426.5
$TiCl_4$	−1000.5	−925.2	−999.2	−993.9	−906.0	−844.5	−851.1	−898.1
$Ti(CO)_4$	−6517.4	−10816.7	−6509.0	−6590.6	−6255.1	−6016.5	−5949.7	−6095.8
TiF_4	−72.0	65.6	−71.0	−83.2	−40.3	31.1	−9.6	−45.0
TiH_4	−2806.3	−2643.4	−2803.9	−2799.6	−2633.3	−2581.7	−2653.5	−2730.7
TiO_2	−356.3	−319.0	−355.2	−350.4	−297.6	−238.6	−255.2	−296.5
TiS_2	−1813.6	−1900.3	−1811.7	−1805.9	−1680.2	−1652.1	−1616.4	−1689.6
VH_5	−5304.3	−5796.8	−5300.0	−5294.3	−5121.9	−4888.2	−4954.6	−5071.1
Zn_2	2457.3	2470.6	2457.4	2474.0	2463.0	2464.4	2463.9	2459.4
$ZnCl_2$	1634.7	1696.1	1635.3	1655.8	1692.1	1811.0	1764.7	1753.7
ZnF_2	1644.0	1729.0	1644.1	1639.1	1635.1	1799.3	1779.0	1756.8
ZnH_2	1577.9	1645.9	1579.1	1590.9	1634.1	1786.4	1713.8	1712.9
$Zn(CH_3)_2$	1345.3	1436.7	1346.7	1348.0	1408.4	1594.3	1499.6	1493.8

3.2.8 Group 4p

Table 24 NMR isotropic shielding constants of various molecules containing 4p elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
As_4	2248.8	2323.5	2249.5	2252.4	2248.3	2256.5	2243.2	2255.1
As_4S_4	1380.5	1402.4	1380.6	1412.4	1383.4	1493.3	1410.1	1457.1
$AsCl_3$	456.3	576.5	456.5	430.4	436.4	500.7	406.3	448.6
AsH_3	1871.9	1908.7	1872.7	1870.8	1863.2	1929.3	1856.2	1900.1
Br_2	1441.8	1576.7	1440.4	1372.1	1373.2	1394.1	1361.7	1363.2
BrCl	776.1	904.9	777.8	659.4	707.2	762.5	686.6	714.8
GaCl	1671.6	1739.9	1672.1	1680.7	1679.9	1704.9	1658.5	1679.9
$GaCl_3$	1348.2	1412.8	1348.8	1374.2	1354.3	1457.4	1374.6	1416.9
GaF	1941.3	1998.3	1942.0	1921.9	1926.1	1956.7	1920.8	1952.8
GaH_3	1045.9	1153.8	1047.6	1075.8	1053.7	1161.6	1068.1	1114.7
$GeCl_4$	1143.4	1208.3	1143.7	1145.9	1119.5	1234.8	1134.7	1186.7
GeF_4	1418.3	1492.5	1419.2	1406.2	1411.5	1555.0	1420.9	1512.8
GeH_4	1614.8	1659.6	1615.4	1630.5	1610.2	1688.7	1625.8	1661.1
GeO	901.7	880.4	902.9	928.4	899.9	1073.4	942.6	1012.9
GeO_2	1374.8	1304.0	1375.6	1401.7	1371.8	1526.7	1406.0	1477.2
HBr	2547.1	2576.0	2548.3	2515.3	2502.7	2523.7	2516.3	2522.4
$CHBr_3$	1256.1	1415.0	1256.6	1276.6	1211.7	1364.2	1323.8	1332.4
KBr	2907.3	2929.9	2883.7	3070.6	3040.7	2975.8	2983.5	2987.3
$PdBr_2$	2498.0	3168.1	2501.8	2463.8	2429.6	2452.2	2437.9	2450.1
$PoBr_2$	2163.5	2378.0	2164.3	2164.4	2138.8	2157.2	2158.4	2155.4
Kr_2	3289.3	3291.3	3289.2	3298.1	3262.6	3263.3	3288.8	3291.0
Se_8	822.4	856.9	822.0	847.3	809.9	912.4	850.0	863.2
SeH_2	2046.2	2080.3	2047.9	2003.6	2007.0	2047.3	2004.7	2024.5
SeO_2	−467.2	−719.5	−466.1	−425.5	−463.9	−277.1	−392.2	−375.8

3.2.9 Group 5s

Table 25 NMR isotropic shielding constants of various molecules containing 5s elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Rb_2	3331.1	3313.6	3330.4	3330.7	3302.0	3349.0	3338.3	3356.4
RbF	3339.1	3343.8	3337.9	3341.2	3293.7	3334.4	3364.5	3370.3
RbH	3238.5	3216.6	3236.4	3220.1	3181.1	3239.3	3252.3	3256.9
Sr_4	3199.2	3278.4	3199.7	3238.4	3501.1	3138.0	3176.7	3169.3
SrF_2	3089.8	3143.4	3089.7	3071.5	3029.4	3189.5	3159.5	3181.7
SrH_2	2597.5	2619.3	2597.6	2583.6	2516.0	2650.1	2613.7	2639.5
SrO	3162.8	3291.1	3162.4	3161.2	3515.1	3183.1	3177.6	3222.2
SrS	2989.1	3101.8	2989.1	2979.6	3543.8	2984.3	2992.7	3013.2

3.2.10 Group 4d

Table 26 NMR isotropic shielding constants of various molecules containing 4d elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Ag_2	4585.5	4593.2	4585.1	4627.8	4541.6	4509.7	4587.8	4565.4
AgCl	4175.9	4167.9	4176.6	4214.2	4123.3	4141.5	4211.6	4190.7
Cd_2	4848.0	4860.7	4847.8	4869.5	4792.8	4761.8	4847.6	4826.9
Cd_2Cl_2	3613.0	3642.7	3612.9	3664.1	3613.7	3551.5	3600.5	3557.4
CdF_2	3856.9	3902.1	3856.2	3865.0	3734.0	3767.4	3830.0	3800.5
$Cd(CH_3)_2$	3040.4	3111.9	3040.2	3078.8	3047.0	2975.1	2987.4	2947.3
Mo_2	−4392.5	−9253.5	−4388.6	−4358.5	−3849.0	−4180.8	−4325.3	−4106.2
$Mo(CO)_6$	1253.4	1219.3	1254.7	1294.9	1374.9	1356.0	1322.2	1361.9
MoO_3	−1185.8	−1331.7	−1181.3	−1194.6	−911.2	−1007.8	−1219.0	−1048.1
NbO_2F	240.3	312.0	244.1	229.5	438.3	371.2	227.3	362.1
$PdBr_2$	−3167.6	−4533.9	−3167.2	−3322.5	−3109.1	−3148.8	−3244.0	−3113.2
$Pd(CO)_4$	292.4	370.4	294.5	420.7	486.7	497.5	412.3	489.4
$Ru(CO)_5$	200.8	−11.7	203.8	271.7	365.3	405.6	311.5	400.1
RuO_2	−4042.1	−4911.7	−4027.1	−4078.2	−3681.0	−3912.2	−4132.8	−3985.5
RuO_4	−2548.0	−3094.1	−2546.9	−2459.2	−2141.1	−2128.1	−2399.4	−2184.9
Tc_2O_7	−1849.9	−2233.2	−1848.3	−1822.5	−1509.2	−1561.0	−1804.9	−1649.8
TcO_3F	−1844.4	−2218.2	−1842.6	−1806.6	−1502.7	−1579.1	−1802.0	−1664.2
YF	2926.3	3033.4	2926.6	2942.8	2961.0	2880.6	2907.3	2215.0
YF_3	2439.0	2589.0	2441.5	2430.4	2466.5	2410.2	2371.9	2177.7
ZrO	2035.1	−28471.2	2037.1	2056.5	2170.8	1993.5	2016.7	2062.9
ZrO_2	1405.4	1622.3	1409.0	1409.3	1544.6	1403.6	1361.9	1447.9

3.2.11 Group 5p

Table 27 NMR isotropic shielding constants of various molecules containing 5p elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
HI	4358.3	4419.1	4362.9	4286.3	4214.7	4306.1	4314.5	4334.1
I_2	2859.1	3112.6	2865.9	2651.4	2598.2	2725.5	2639.2	2673.8
ICl	−307.4	−12.4	−277.9	−579.5	−558.0	−44.5	−403.4	−258.3
InCl	3487.6	3606.7	3498.3	3476.4	3399.0	3434.9	3412.9	3413.6
$InCl_3$	2908.7	3000.8	2918.7	2919.2	2839.6	3028.2	2917.0	2956.7
InH	1803.0	2005.8	1839.6	1806.2	1714.3	1843.9	1696.5	1729.2
InH_3	2271.5	2445.3	2294.0	2302.5	2210.4	2423.4	2298.0	2337.4
KI	5373.4	5406.8	5336.6	5573.6	5470.9	5479.3	5532.5	5548.8
SbF_3	2161.7	2380.9	2163.6	2005.6	1940.9	2158.9	2036.4	2195.0
SbH_3	3269.2	3337.2	3272.3	3294.3	3239.3	3452.1	3361.7	3403.0
SnH_4	3007.8	3087.1	3013.2	3036.6	2987.1	3217.7	3146.4	3177.7
SnO	1756.8	1625.9	1766.3	1753.7	1656.1	2004.5	1845.3	1905.7
SnO_2	3017.1	2721.1	3022.2	2994.8	2875.6	3202.4	3080.7	3146.7
TeH_2	3427.1	3495.0	3433.8	3361.3	3333.8	3494.9	3403.7	3459.7
TeO_2	−488.3	−1103.5	−488.4	−456.9	−516.0	−37.5	−387.4	−283.0
XeF_2	2064.5	1940.6	2073.4	2941.5	2713.7	2985.1	2935.4	2810.2
XeF_4	−739.7	−424.5	−715.1	−89.9	−236.1	195.3	−24.9	−24.7
$XeOF_4$	−474.2	−443.9	−459.6	−321.8	−318.6	−48.7	−231.6	−113.0

3.2.12 Group 6s

Table 28 NMR isotropic shielding constants of various molecules containing 6s elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Ba_4	5403.8	5662.5	5319.8	5546.9	5982.6	5486.6	5612.3	5605.6
BaF_2	5580.5	5665.6	5581.2	5559.9	5266.9	5556.6	5669.3	5694.0
BaH_2	4531.0	4614.7	4519.9	4553.4	4479.8	4632.7	4709.6	4727.4
BaO	5427.0	5671.4	5439.9	5503.2	4813.2	5449.2	5575.4	5586.0
BaS	4931.2	5200.3	4921.0	5000.8	5261.3	5008.3	5126.7	5127.3
Cs_2	5845.2	5814.6	5844.2	5853.9	5712.7	5805.8	5923.2	5928.3
CsF	5882.7	5908.7	5886.2	5913.3	5683.7	5729.8	5884.8	5918.5
CsH	5672.4	5658.8	5675.6	5671.9	5507.9	5644.3	5769.7	5764.8

3.2.13 Group 5d

Table 29 NMR isotropic shielding constants of various molecules containing 5d elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
Au_2	9723.2	9809.3	9723.5	9832.3	9156.9	9356.1	9871.4	9863.0
AuCl	8516.6	8567.5	8516.5	8573.2	7931.0	8455.2	8985.5	8966.3
HfO	6305.6	6732.0	6306.4	6338.5	6349.7	5599.4	5907.2	5931.7
HfO_2	4644.6	5294.7	4650.3	4644.6	4725.0	4087.5	4352.5	4424.7
Hg_2	10518.9	10532.7	10518.3	10577.4	9955.3	9920.1	10473.5	10458.1
Hg_2Cl_2	7974.9	7968.0	7974.5	8085.4	7639.5	8283.4	8632.4	8732.0
HgF_2	8040.4	8089.6	8040.2	8104.2	7531.2	8150.4	8644.4	8658.6
$Hg(CH_3)_2$	6435.2	6523.4	6436.1	6520.0	6296.0	7130.2	7464.0	7593.1
$LaCl_3$	3729.4	4001.3	3744.4	3630.3	2985.3	3973.2	3950.1	4077.5
LaF_3	4849.9	5043.4	4871.6	4767.1	4286.3	4887.6	4939.0	4979.9
LaH_3	2271.4	2575.0	2268.2	2180.0	1610.5	2320.6	2259.5	2411.1
$Os(CO)_5$	3115.7	3076.5	3119.1	3217.5	3088.5	3054.5	3441.8	3477.0
OsO_3	−5493.8	−6066.2	−5488.7	−5410.7	−4765.5	−5487.1	−5535.3	−5387.7
OsO_4	−1617.5	−1991.8	−1613.0	−1532.3	−1195.8	−1626.1	−1531.3	−1397.6
$Pt(CO)_4$	3097.7	3220.1	3099.5	3276.9	3076.7	3208.1	3531.6	3576.7
PtO_2	−3311.7	−4854.7	−3297.5	−3312.4	−2874.7	−2296.4	−2266.0	−2177.1
Re_2O_7	−478.2	−651.4	−478.9	−474.8	−165.5	−657.4	−579.2	−419.2
TaF_3	−5215.6	−7371.5	−5206.4	−4906.5	−3665.7	−6453.0	−5914.7	−6347.6
TaO_2F	1410.0	1865.0	1414.4	1419.7	1618.2	1296.1	1552.2	1607.2
$W(CO)_6$	4515.4	4632.9	4517.6	4595.6	4407.9	4404.9	4930.9	4860.3
WO_3	−2138.8	−2040.2	−2134.3	−2130.7	−1755.2	−2100.3	−1872.4	−1807.5

3.2.14 Group 6p

Table 30 NMR isotropic shielding constants of various molecules containing 6p elements.

Molecule	ET	ANO-RCC PBE0	ANO-RCC	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
At_2	4691.7	5243.9	4675.2	4010.9	3406.6	3672.3	4163.4	4087.9
AtCl	−3156.6	−2741.3	−3167.2	−4021.5	−4655.8	−3740.2	−3753.5	−3626.5
AtF_3	−7551.9	−7391.1	−7561.3	−6643.5	−7346.3	−6338.4	−6328.6	−6833.6
BiF_3	4865.3	5354.1	4874.2	4429.3	3817.6	4107.6	4506.3	4736.2
BiH_3	6663.7	6790.4	6668.7	6727.0	6125.3	6231.0	6790.5	6715.8
PbH_4	6479.6	6619.3	6493.8	6525.9	5954.7	6140.2	6713.5	6617.8
PbO	3590.3	3099.4	3609.3	3482.2	2821.4	3068.5	3528.5	3586.1
PbO_2	6826.9	5893.9	6836.1	6794.3	6032.6	6232.6	6794.3	6812.8
$PoBr_2$	−7457.3	−6376.2	−7489.4	−8652.7	−9367.7	−8526.7	−8357.2	−8542.2
$PoCl_4$	454.3	793.0	464.5	174.6	−219.8	128.8	536.4	305.5
PoF_2	−12237.8	−11563.0	−12256.7	−11560.1	−12405.8	−11393.6	−11330.9	−11949.9
PoF_6	4365.7	4447.6	4373.1	4034.4	3472.2	3921.0	4423.2	4405.1
PoO_2	−1544.2	−3910.6	−1535.0	−1518.9	−2118.8	−1712.2	−1416.7	−1566.1
Rn_2	10093.2	10128.1	10099.7	10229.0	9431.6	9475.0	10207.3	10098.1
RnF_2	−1513.3	−2032.8	−1528.4	1740.1	154.4	1050.9	1354.5	436.8
TlCl	7600.9	7888.4	7624.1	7501.7	6906.7	6892.3	7394.9	7354.1
$TlCl_3$	6472.2	6528.9	6492.1	6467.6	5842.2	6001.7	6452.1	6441.7
TlH	4032.1	4432.6	4090.5	3967.4	3309.7	3532.1	3878.6	3906.2
TlH_3	4618.3	4881.7	4656.9	4647.3	4002.1	4327.5	4743.6	4722.2

3.3 Statistical evaluation

The individual shielding constants are evaluated statistically. Only symmetry non-equivalent nuclei are considered. For details see main text.

Table 31 Mean absolute error and standard deviation of various triple-ζ basis sets and the uncontracted ANO-RCC bases compared to the large even-tempered reference.

Group	n_g	ANO-RCC	Dyall-VTZ	Sapporo-TZP	TZVPall	TZVPPall	TZVPall-2c	TZVPall-s
1s	93	0.1 ±0.3	0.2 ±0.3	0.2 ±0.4	0.4 ±0.4	0.3 ±0.4	0.4 ±0.4	0.3 ±1.1
2s	19	0.9 ±0.5	0.2 ±0.2	5 ±4	2 ±2	2 ±2	2 ±2	1.1 ±0.9
2p	194	2 ±6	11 ±9	12 ±14	11 ±9	11 ±9	11 ±9	5 ±6
3s	14	0.2 ±0.1	1.1 ±0.6	2 ±4	2.7 ±1.1	2.7 ±0.9	0.8 ±0.7	0.8 ±0.7
3p	76	4 ±11	14 ±19	13 ±19	15 ±15	14 ±14	12 ±14	11 ±13
4s	12	29 ±33	31 ±44	26 ±34	15 ±15	16 ±16	11 ±17	11 ±16
3d	27	3 ±4	22 ±32	72 ±76	68 ±59	67 ±58	69 ±57	30 ±26
4p	24	2 ±5	8 ±12	12 ±8	24 ±20	21 ±18	22 ±16	19 ±17
5s	8	0.7 ±0.7	10 ±13	54 ±38	18 ±10	14 ±12	6 ±5	13 ±12
4d	21	2 ±3	11 ±11	141 ±113	51 ±33	47 ±30	20 ±25	47 ±45
5p	18	13 ±12	45 ±73	66 ±28	65 ±42	62 ±40	35 ±38	36 ±28
6s	8	16 ±28	10 ±12	78 ±54	144 ±11	140 ±26	18 ±24	28 ±19
5d	21	5 ±6	25 ±37	378 ±259	335 ±173	355 ±169	48 ±46	63 ±52
6p	19	18 ±13	111 ±184	657 ±159	492 ±189	492 ±191	138 ±124	84 ±103

Table 32 Mean absolute error and standard deviation of various double-ζ basis sets compared to the large even-tempered reference.

Group	n_g	Dyall-VDZ	Sapporo-DZP	SVPall	SVPall-2c	SVPall-s
1s	93	0.4 ±0.4	0.6 ±0.7	0.6 ±0.5	0.6 ±0.5	0.5 ±1.1
2s	19	1.3 ±1.1	5 ±3	4 ±5	4 ±5	1.5 ±1.5
2p	194	25 ±25	39 ±103	31 ±24	18 ±24	20 ±25
3s	12	2 ±2	3 ±3	23 ±11	3.3 ±1.7	4 ±2
3p	76	29 ±40	40 ±133	57 ±65	38 ±37	34 ±38
4s	12	42 ±52	37 ±46	40 ±23	23 ±22	25 ±20
3d	27	28 ±36	115 ±93	245 ±152	205 ±150	159 ±129
4p	24	34 ±38	27 ±32	75 ±55	36 ±27	54 ±34
5s	8	13 ±13	185 ±194	33 ±35	22 ±21	40 ±25
4d	21	42 ±40	173 ±152	128 ±107	52 ±40	153 ±161
5p	18	157 ±239	167 ±167	253 ±274	178 ±234	187 ±215
6s	8	47 ±48	298 ±206	66 ±46	125 ±71	135 ±63
5d	21	79 ±70	428 ±350	315 ±354	358 ±305	417 ±352
6p	19	486 ±762	836 ±461	709 ±528	459 ±679	325 ±489

3.4 Weighted Overall Error

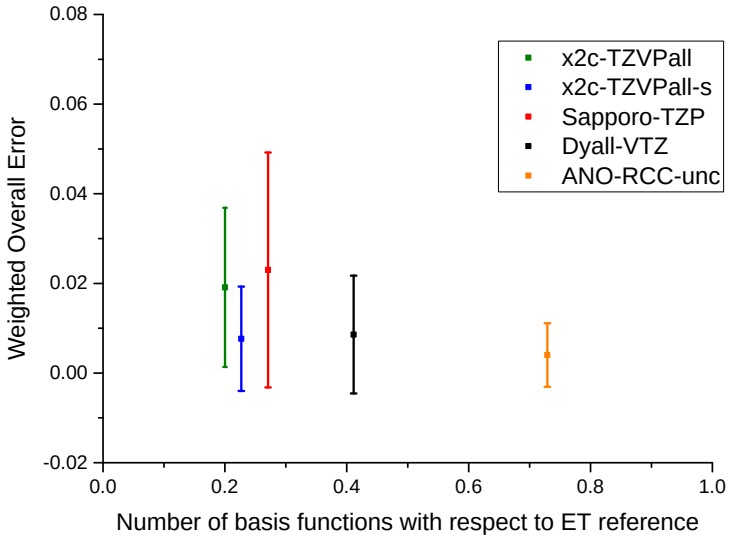

Fig. 2 Weighted overall error of triple-ζ and ANO-RCC-unc bases compared to the total number of contracted basis functions in the spherical atomic orbital (AO) basis.

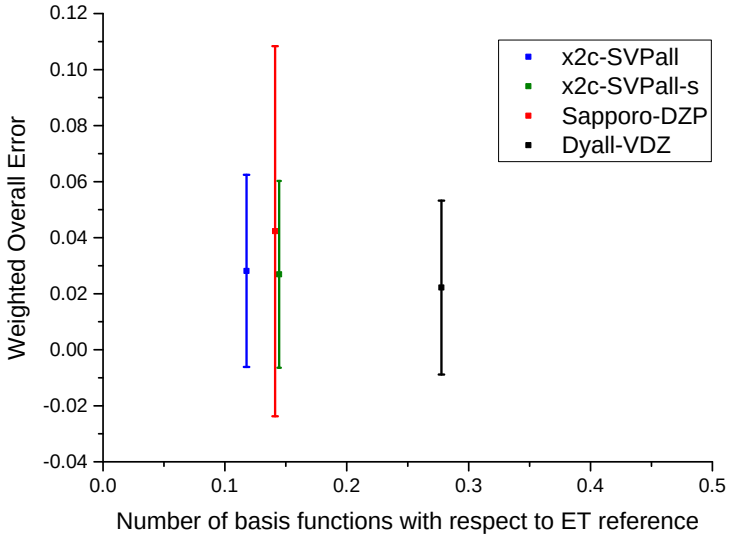

Fig. 3 Weighted overall error of double-ζ bases compared to the total number of contracted basis functions in the spherical atomic orbital (AO) basis.

The weighted errors (see main text) of the triple-ζ and double-ζ bases are displayed in Fig. 2 and 3, respectively. The triple-ζ basis sets are discussed in the main text. So, we will only consider the double-ζ basis sets here. The Sapporo-DZP, the x2c-SVPall and the x2c-SVPall-s bases employ roughly the same number of functions, while the uncontracted Dyall-VDZ basis set is very large compared to them. But, the Dyall-VDZ basis sets also yields the smallest error. The Sapporo bases show a very large standard deviation and the largest error of all chosen basis sets. The extensions of the x2c-SVPall-s bases result in only a minor improvement compared to the x2c-SVPall set. The main improvement is found for the 6p group (see Tab. 32), where the unmodified x2c-SVPall set results in an error of 709 ppm.

4 Comparison with pcSseg bases

4.1 Group 1s

Table 33 NMR isotropic shielding constants of various molecules containing 1s elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
AlH_3	25.5	25.8	25.4	25.5	25.5	25.5	25.4	25.5
AsH_3	28.6	29.6	28.6	28.6	28.6	28.6	28.5	28.6
B_2H_6	31.4	32.2	31.5	31.5	31.4	31.4	31.5	31.4
B_2H_6	26.3	27.1	26.3	26.3	26.3	26.3	26.4	26.3
$B_3N_3H_6$	26.1	26.8	26.3	26.1	26.1	26.1	26.4	26.2
$B_3N_3H_6$	25.0	27.2	25.1	25.1	25.0	25.0	25.1	25.2
B_4H_4	19.9	20.4	19.9	20.0	19.9	19.9	20.1	19.9
Be_2H_4	25.8	26.5	26.0	25.9	25.8	25.9	26.0	25.7
Be_2H_4	26.0	26.5	26.3	26.4	26.4	26.4	26.4	25.5
BeC_2H_6	31.7	32.9	31.6	31.6	31.6	31.6	31.7	31.8
$BeF_2O_2H_4$	28.2	30.8	28.6	28.3	28.1	28.1	28.8	28.6
BeH_2	27.4	27.7	27.7	27.9	27.9	28.0	27.7	26.6
BH_3	22.7	23.4	22.7	22.7	22.7	22.7	22.7	22.8
BH_3CO	29.5	30.0	29.3	29.4	29.4	29.4	29.5	29.5
BH_3NH_3	28.8	29.4	28.7	28.8	28.8	28.8	28.9	28.9
BH_3NH_3	28.1	30.5	28.5	28.2	28.1	28.1	28.4	28.4
C_2H_2	29.7	30.3	29.5	29.7	29.6	29.6	29.8	29.6
C_2H_3N	30.9	31.9	31.3	31.0	30.8	30.8	31.2	31.1
C_2H_3N	23.7	25.0	23.7	23.7	23.6	23.6	23.9	23.6
C_2H_4	25.2	27.0	25.4	25.2	25.2	25.2	25.5	25.3
C_2H_6	30.0	31.4	30.0	30.0	30.0	30.0	30.1	30.1
C_4H_4	28.0	29.7	28.1	28.0	27.9	27.9	28.4	28.1
C_6H_6	23.4	25.8	23.7	23.4	23.4	23.4	23.9	23.6
CaH_2	26.0	25.6	25.7	25.9	25.9	25.9	25.6	25.7
CH_2O	20.5	21.9	20.9	20.6	20.4	20.4	21.2	20.7
CH_2O_2	25.9	26.9	25.8	25.9	25.8	25.8	26.0	25.9
CH_3N	20.3	21.3	20.1	20.2	20.2	20.2	20.1	20.4
CH_3N	22.5	24.2	22.9	22.6	22.5	22.4	23.2	22.7
CH_4	23.0	24.3	23.3	23.1	23.0	22.9	23.5	23.2
CuH	30.8	31.9	30.7	30.8	30.8	30.8	30.8	30.9
Ferrocene	33.3	50.2	35.5	33.9	33.4	33.2	32.6	33.4
GaH_3	27.0	29.2	27.2	27.1	27.0	27.0	27.3	27.2
GeH_4	24.2	24.9	24.3	24.2	24.2	24.2	24.1	24.3
H_2	27.1	28.5	27.2	27.2	27.1	27.1	27.1	27.1
H_2CO_3	26.2	26.5	26.0	26.2	26.2	26.2	26.0	26.2
H_2O	25.8	28.3	26.2	25.8	25.7	25.7	26.3	26.1
H_2O_2	30.8	32.6	30.9	30.8	30.7	30.7	31.1	31.0
H_2SO_4	24.3	26.4	24.6	24.4	24.2	24.2	24.9	24.6
H_3PO_4	26.1	28.7	26.5	26.2	26.0	26.0	26.8	26.4
$CHBr_3$	27.5	30.5	27.9	27.6	27.4	27.4	28.2	27.8
HCl	31.1	32.8	30.9	30.9	31.0	31.0	31.2	31.0
HCN	22.4	25.1	22.4	22.6	22.3	22.3	22.8	22.6
HCP	30.7	32.4	30.5	30.6	30.7	30.7	31.0	30.7
He_2	28.3	28.6	28.2	28.3	28.2	28.2	28.7	28.2
HF	28.8	28.8	28.5	28.7	28.8	28.8	28.8	28.7
HNC	59.9	59.3	59.6	59.7	59.7	59.7	59.7	59.8
HNO	27.1	31.1	29.4	29.3	29.2	29.2	27.3	27.0
HNO_2	27.1	27.3	26.9	27.1	27.0	27.0	27.3	27.0
HNO_3	27.1	27.3	26.9	27.1	27.0	27.0	27.3	27.0

H_2S	16.3	18.0	16.9	16.5	16.2	16.2	17.1	16.6
H_2S_2	21.2	23.2	21.7	21.3	21.2	21.1	22.0	21.5
KH	30.3	32.0	30.2	30.2	30.2	30.2	30.6	30.3
$Li_4C_4H_{12}$	27.5	29.9	27.7	27.5	27.4	27.4	28.1	27.6
Li_4H_4	24.9	24.5	24.6	24.8	24.8	24.9	24.7	24.8
$LiBH_4$	32.6	33.5	32.5	32.6	32.6	32.6	32.6	32.7
$LiBH_4$	27.7	27.6	27.6	27.7	27.7	27.7	27.6	27.8
LiH	30.2	30.5	30.0	30.2	30.2	30.2	30.2	30.2
MgH_2	31.3	31.8	31.1	31.3	31.3	31.3	31.3	31.4
H_2N_2	26.1	25.9	25.9	26.0	26.1	26.2	25.8	26.0
N_2H_4	26.5	26.4	26.4	26.4	26.4	26.5	26.2	26.3
N_2H_4	14.3	14.0	14.4	14.3	14.3	14.2	14.4	14.6
NaH	28.0	30.6	28.6	28.1	28.0	28.0	28.8	28.4
NH_3	28.2	30.3	28.6	28.2	28.1	28.1	28.8	28.5
NH_3HF	25.6	25.2	25.4	25.5	25.6	25.6	25.4	25.5
NH_3HF	31.3	33.0	31.4	31.3	31.2	31.2	31.5	31.5
PbH_4	30.3	31.8	30.3	30.3	30.2	30.2	30.4	30.5
PH_3	22.0	24.9	22.0	22.0	21.8	21.8	22.1	22.1
SbH_3	29.1	30.3	29.0	29.0	29.0	29.0	29.1	29.1
ScH_3	24.0	23.6	24.1	24.2	24.0	24.0	24.7	24.1
SeH_2	29.9	31.5	29.9	29.9	29.9	29.9	30.1	30.0
SiH_4	27.4	29.1	27.5	27.4	27.4	27.4	27.5	27.4
TiH_4	19.4	18.3	19.2	19.3	19.4	19.5	18.6	19.2
VH_5	10.8	11.1	10.3	10.5	10.8	10.8	9.6	10.2
VH_5	15.2	15.2	15.2	15.2	15.2	15.2	14.6	15.0
ZnH_2	26.7	27.1	26.6	26.7	26.7	26.7	26.3	26.6
$Zn(CH_3)_2$	31.2	32.5	31.2	31.2	31.1	31.1	31.2	31.3

4.2 Group 2s

Table 34 NMR isotropic shielding constants of various molecules containing 2s elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
Be_2F_4	103.6	105.4	105.2	103.0	101.9	101.7	105.7	105.5
Be_2H_4	79.7	80.9	81.3	79.0	78.2	78.2	82.3	82.2
Be_4	139.5	135.2	137.8	138.7	138.6	138.7	136.7	140.6
BeC_2H_6	70.6	75.1	72.4	70.2	69.1	69.0	72.9	73.0
$BeF_2O_2H_4$	104.6	107.6	106.7	104.2	103.1	102.9	107.8	106.3
BeH_2	75.4	77.2	76.2	74.4	73.7	73.7	77.9	78.7
BeS	97.4	95.3	96.4	96.8	96.1	95.9	91.0	99.6
Li_2	98.6	98.3	98.6	98.4	98.4	98.4	98.2	98.9
Li_2O	84.3	84.3	84.4	83.8	83.7	83.6	83.3	84.7
$Li_4C_4H_{12}$	85.0	85.6	85.5	84.6	84.4	84.4	84.9	85.5
Li_4Cl_4	88.6	89.5	89.7	88.6	88.0	88.0	89.3	89.3
Li_4H_4	87.2	87.1	87.3	86.7	86.6	86.6	86.9	87.9
Li_8	101.3	100.7	101.3	100.9	100.9	100.9	100.6	101.8
$LiBH_4$	90.3	91.1	90.9	90.0	89.9	89.8	90.2	90.7
LiCl	87.6	87.0	87.8	86.9	86.9	86.8	86.7	87.8
LiF	87.3	86.4	86.9	86.7	86.5	86.4	86.1	87.6
LiH	89.2	88.7	89.2	88.6	88.6	88.6	89.0	89.7
Li_2S	86.2	85.7	86.2	85.5	85.4	85.3	84.7	86.1
Li_3P	89.7	89.4	89.8	89.1	89.0	89.0	89.2	90.3

4.3 Group 2p

Table 35 NMR isotropic shielding constants of various molecules containing 2p elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
Al_2O_3	291.2	353.6	301.3	291.2	291.2	291.2	311.9	293.7
Al_2O_3	217.8	149.6	199.0	208.2	218.3	218.6	193.1	214.7
AlF_3	378.4	382.3	360.4	374.2	378.0	378.2	412.3	382.8
B_2H_6	72.2	74.0	75.3	72.3	72.2	72.2	74.7	74.6
$B_3N_3H_6$ (B)	65.7	76.0	69.1	65.9	65.6	65.6	69.5	68.2
$B_3N_3H_6$ (N)	103.2	111.5	105.4	103.5	103.3	103.2	108.9	105.8
B_4H_4	−81.6	−80.3	−75.6	−81.9	−81.5	−81.5	−75.6	−76.5
Be_2F_4	347.4	393.6	361.6	347.0	347.2	347.2	386.5	351.6
Be_2F_4	355.5	315.3	348.4	352.9	355.1	355.3	365.1	357.3
BeC_2H_6	192.6	198.0	191.5	192.6	192.6	192.6	192.2	193.5
$BeF_2O_2H_4$ (F)	368.7	344.7	360.9	365.1	368.8	368.6	393.0	374.2
$BeF_2O_2H_4$ (O)	283.0	296.7	286.8	282.9	283.0	283.0	291.7	283.6
BF_3 (B)	82.2	88.4	83.2	82.4	82.0	82.0	85.8	84.0
BF_3 (F)	289.0	273.3	281.3	287.1	289.0	289.1	308.3	292.4
BH_3	−7.8	−5.1	−3.0	−8.0	−7.9	−7.8	−4.5	−3.8
BH_3CO (B)	157.1	160.3	157.8	157.2	157.0	157.0	158.5	158.0
BH_3CO (C)	−18.6	−13.3	−13.5	−18.4	−18.5	−18.6	−11.8	−14.8
BH_3CO (O)	−47.4	−69.8	−50.3	−47.8	−47.1	−47.2	−47.4	−44.8
BH_3NH_3 (B)	116.9	123.9	118.4	116.8	116.9	116.9	119.7	118.9
BH_3NH_3 (N)	216.2	223.4	215.2	216.0	216.2	216.2	216.7	217.2
C_2H_2	104.5	110.0	106.8	104.5	104.6	104.5	106.3	106.9
C_2H_3N (N)	225.4	217.4	222.9	225.4	225.5	225.5	223.6	226.5
C_2H_3N (C)	53.5	57.0	56.6	53.4	53.6	53.5	56.8	56.6
C_2H_4	43.4	52.9	47.5	43.5	43.5	43.4	47.2	46.8
C_2H_6	167.4	176.2	168.1	167.5	167.4	167.4	168.4	169.2
C_4H_4	204.0	204.8	203.7	204.1	204.0	203.9	203.9	204.6
C_6H_6	40.0	52.0	45.7	40.3	40.0	40.0	46.6	43.6
CaF_2	159.9	209.1	98.7	140.9	159.5	159.2	245.2	174.5
CF_4 (C)	35.1	31.3	40.7	35.1	35.1	35.0	43.1	38.5
CF_4 (F)	216.9	222.9	221.0	217.1	217.3	217.1	238.3	221.1
CH_2O (C)	−29.4	−20.7	−20.5	−28.9	−29.4	−29.5	−18.8	−24.7
CH_2O (O)	−448.6	−539.7	−474.2	−452.7	−448.1	−447.9	−476.5	−445.2
CH_2O_2 (C)	83.4	86.6	86.3	83.1	83.4	83.3	87.1	85.7
CH_2O_2 (O)	21.6	−5.4	13.8	20.1	21.9	22.0	17.4	24.3
CH_3N (N)	−132.2	−163.1	−136.5	−133.9	−131.9	−131.9	−138.6	−129.1
CH_3N (C)	1.0	11.9	8.2	1.5	1.0	0.9	8.9	5.4
CH_4	185.0	188.4	184.2	184.9	185.0	185.0	183.5	186.1
ClF	629.7	489.6	597.4	619.9	628.9	630.1	600.5	627.7
ClF_3	−182.6	−282.6	−185.3	−175.9	−180.7	−181.6	−173.8	−176.0
ClF_3	21.7	−72.9	6.1	14.7	21.9	22.6	24.4	26.9
CO (C)	−21.9	−18.9	−19.9	−21.9	−21.9	−21.9	−16.8	−18.5
CO (O)	−95.8	−123.8	−99.9	−96.4	−95.6	−95.5	−96.5	−93.0
CO_2 (C)	47.5	53.7	50.0	47.8	47.4	47.4	52.3	50.3
CO_2 (O)	199.0	184.8	195.2	198.0	199.1	199.1	199.6	200.2
$Cr(CO)_6$ (C)	−42.7	−36.9	−36.1	−42.2	−42.6	−42.7	−34.8	−38.8
$Cr(CO)_6$ (O)	−103.0	−129.5	−103.6	−102.7	−102.5	−102.7	−99.9	−99.5
CrO_3	−1446.0	−1562.1	−1493.1	−1453.8	−1442.6	−1441.7	−1495.3	−1443.0
CS_2	−24.5	−16.9	−16.2	−24.2	−24.2	−24.4	−13.5	−19.6
Cu_2O	582.3	887.1	663.5	590.8	583.6	579.8	577.2	579.6
CuCN (C)	68.7	74.2	75.3	69.2	68.7	68.7	76.5	73.2
CuCN (N)	−119.3	−154.1	−123.2	−120.3	−119.3	−119.2	−122.8	−117.2

CuF	677.1	1252.4	756.6	693.4	679.5	674.4	711.5	685.2
F_2	−274.9	−305.4	−276.9	−272.5	−271.0	−272.9	−289.8	−272.9
$Fe(CO)_5$ (C)	−45.6	−40.9	−38.7	−45.1	−45.5	−45.6	−37.0	−41.2
$Fe(CO)_5$ (C)	−60.4	−60.0	−54.3	−60.0	−60.2	−60.3	−51.4	−56.2
$Fe(CO)_5$ (O)	−103.6	−127.7	−102.3	−103.2	−103.2	−103.3	−98.0	−100.0
$Fe(CO)_5$ (O)	−137.2	−172.2	−138.8	−137.3	−136.7	−136.9	−131.7	−133.6
Ferrocene	99.8	108.8	103.3	100.0	99.9	99.8	103.2	102.4
GaF	72.4	−45.8	29.1	66.0	72.2	73.3	82.8	78.1
GeF_4	298.0	289.6	283.7	295.4	299.4	299.3	315.0	301.2
GeO	−424.7	−526.6	−445.4	−434.4	−425.0	−423.6	−465.6	−432.8
GeO_2	−51.4	−183.3	−57.6	−53.6	−48.7	−49.0	−71.5	−52.4
H_2CO_3 (C)	13.6	19.3	19.0	13.7	13.5	13.4	22.3	17.4
H_2CO_3 (O)	12.2	−2.7	9.6	11.8	12.4	12.3	13.4	16.4
H_2CO_3 (O)	147.1	153.8	151.2	147.8	147.2	147.1	158.4	151.0
H_2O	318.4	323.2	326.4	320.0	318.8	318.8	330.0	318.8
H_2O_2	84.1	56.8	78.8	83.4	84.4	84.4	82.5	85.4
H_2SO_4 (O)	19.5	−10.3	17.5	20.3	19.7	19.5	23.9	23.7
H_2SO_4 (O)	81.5	86.7	87.7	81.9	81.7	81.6	99.4	85.3
H_3PO_4	193.6	215.4	199.9	193.6	193.6	193.6	209.7	197.4
$H_3\ PO_4$	150.1	142.7	141.6	148.8	150.0	149.9	151.4	151.7
$CHBr_3$	54.5	71.1	58.2	54.2	54.4	54.5	59.4	57.4
HCN (C)	67.1	67.5	70.5	67.3	67.2	67.1	70.9	69.7
HCN (N)	−52.8	−55.2	−53.1	−53.6	−52.6	−52.7	−55.7	−49.7
HCP	10.3	10.2	14.0	9.9	10.5	10.4	14.6	13.9
HF	403.4	401.2	401.1	401.7	403.1	403.4	434.1	409.3
HNC (N)	85.6	82.6	89.4	85.7	85.8	85.7	88.5	88.1
HNC (C)	1.3	13.1	3.7	1.1	1.3	1.3	3.5	5.0
HNO (O)	−2126.4	−2810.1	−2242.7	−2144.1	−2129.8	−2123.6	−2314.9	−2121.8
HNO (N)	−1052.9	−1353.3	−1089.0	−1062.5	−1054.8	−1051.6	−1117.0	−1041.9
HNO_2 (N)	−121.2	−121.2	−109.6	−120.5	−121.1	−121.3	−103.8	−115.3
HNO_2 (O)	−375.0	−458.2	−381.6	−376.3	−374.4	−374.3	−380.3	−369.7
HNO_3 (N)	−98.9	−101.4	−87.4	−98.7	−98.8	−99.0	−82.2	−93.8
HNO_3 (O)	−199.5	−233.8	−195.9	−198.8	−199.1	−199.3	−186.4	−192.6
HNO_3 (O)	−101.0	−131.1	−103.6	−101.2	−100.7	−100.8	−91.6	−97.0
HNO_3 (O)	−194.3	−239.3	−187.3	−193.8	−193.7	−193.8	−184.5	−187.2
KF	296.2	225.4	168.8	235.8	263.6	266.6	377.3	314.5
Li_2O	159.9	150.1	157.9	158.1	159.2	159.7	180.4	180.2
$Li_4C_4H_{12}$	193.6	197.5	194.2	193.6	193.6	193.5	192.9	195.1
$LiBH_4$	142.4	143.7	143.6	142.5	142.4	142.3	142.9	144.6
LiF	341.9	220.8	278.3	321.6	339.1	341.1	366.5	347.2
MgF_2	427.9	446.0	425.4	419.9	426.5	427.4	449.1	427.9
N_2	−98.6	−115.8	−100.9	−99.2	−99.2	−98.5	−94.4	−95.6
N_2H_2	−380.2	−442.3	−375.8	−381.9	−380.1	−380.0	−387.8	−371.5
N_2H_4	185.4	182.1	185.8	185.8	185.6	185.5	186.2	186.0
N_4	206.2	190.0	206.5	206.3	206.3	206.2	207.0	207.7
Na_2O	326.4	848.1	485.8	314.9	329.2	328.1	355.5	334.7
Na_3N	−135.6	−23.8	−79.2	−151.8	558.6	−132.3	−129.8	−131.9
NaF	445.8	410.1	404.9	422.1	442.1	445.2	475.1	445.2
Ne_2	551.0	552.1	551.8	551.0	550.9	551.0	552.5	551.1
NF_3 (N)	−197.8	−217.5	−192.8	−199.2	−197.6	−197.6	−190.7	−192.7
NF_3 (F)	−31.3	−34.5	−12.9	−29.1	−30.0	−30.9	0.4	−23.0
NF_3 (F)	−30.4	−34.0	−12.1	−28.2	−29.2	−30.0	1.2	−22.2
NH_3	254.8	257.6	260.2	256.4	254.9	254.8	259.1	254.8
NH_4F (N)	242.3	242.4	241.9	242.0	242.3	242.3	244.2	242.6
NH_4F (F)	365.1	430.9	392.2	368.7	365.0	364.7	445.4	385.6
$Ni(CO)_4$ (C)	−29.3	−27.0	−23.0	−28.7	−29.2	−29.2	−21.8	−25.1

$Ni(CO)_4$ (O)	−90.7	−115.6	−88.2	−90.4	−90.3	−90.5	−85.4	−87.0
OF_2 (F)	−700.7	−703.9	−690.8	−697.9	−698.5	−699.3	−679.4	−691.5
OF_2 (O)	−122.8	−154.9	−114.3	−119.1	−119.7	−121.6	−116.8	−117.0
PF_3	159.0	169.2	162.4	162.2	159.4	159.0	204.8	166.3
PF_5	184.4	188.8	187.1	186.1	184.3	184.3	219.9	190.9
PF_5	194.6	200.6	192.5	194.4	194.3	194.5	218.4	197.4
ScF_3	−67.5	−173.2	−115.7	−76.3	−65.9	−66.1	−63.0	−70.1
SeO_2	−673.1	−908.6	−693.2	−681.4	−675.3	−673.6	−701.1	−674.0
SF_2	292.7	314.0	306.2	299.2	293.3	292.5	332.7	303.1
SF_4	−9.6	1.3	5.9	−0.8	−8.9	−9.7	37.8	−1.5
SF_4	35.6	17.0	43.3	39.9	36.1	35.9	75.0	42.1
SF_6	6.7	−26.3	8.6	6.9	7.1	7.3	34.9	11.2
SiF_4	324.4	346.2	317.2	323.0	324.1	324.2	355.4	328.5
SiO_2	172.2	66.0	139.9	162.5	172.3	173.1	141.8	170.5
$Ti(CO)_4$ (C)	−428.2	−440.0	−391.1	−425.8	−428.4	−428.2	−399.5	−422.4
$Ti(CO)_4$ (O)	−1225.2	−1308.4	−1180.1	−1221.1	−1225.8	−1225.3	−1227.8	−1229.6
TiF_4	−179.6	−269.7	−221.8	−185.4	−177.9	−178.2	−191.5	−180.5
TiO_2	−829.5	−919.6	−870.3	−837.2	−827.0	−827.9	−851.3	−829.1
ZnF_2	412.4	431.5	408.6	411.3	414.1	413.6	444.1	416.7
$Zn(CH_3)_2$	184.4	197.3	188.5	185.4	184.7	184.5	187.5	186.4

4.4 Group 3s

Table 36 NMR isotropic shielding constants of various molecules containing 3s elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
Mg_4	707.2	700.6	702.6	704.1	704.1	704.3	706.1	706.7
$MgCl_2$	496.9	494.0	491.0	491.9	494.1	494.6	494.3	496.0
MgF_2	538.2	543.0	525.4	535.3	536.0	535.8	534.3	537.7
MgH_2	426.1	447.2	425.9	424.0	423.9	424.0	422.8	424.5
Na_2	610.7	613.2	608.5	609.2	608.4	608.4	612.3	610.4
Na_2O	584.7	568.5	577.6	584.4	582.8	582.3	584.0	582.3
Na_2S	567.6	557.2	561.2	567.2	565.4	565.4	570.8	566.4
Na_3N	588.6	599.8	589.1	588.0	579.6	586.2	590.2	588.3
Na_3P	581.9	587.0	581.1	580.8	579.6	579.5	586.4	581.8
Na_3P	582.0	587.1	581.2	580.9	579.7	579.7	586.5	581.9
Na_3P	582.5	587.7	581.7	581.3	580.2	580.1	587.0	582.3
NaCl	570.1	570.2	566.2	568.1	567.8	567.9	579.5	579.7
NaF	580.1	584.8	575.4	578.5	578.0	577.8	587.4	578.5
NaH	577.3	577.3	574.3	575.3	575.0	575.1	579.3	577.0

4.5 Group 3p

Table 37 NMR isotropic shielding constants of various molecules containing 3p elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
Al_2O_3	478.6	470.3	481.1	477.0	475.1	475.6	469.8	478.7
Al_2S_3 (Al)	379.3	343.4	381.7	375.8	376.0	376.7	371.3	381.0
Al_2S_3 (S)	647.5	644.5	639.2	634.7	641.4	643.4	680.6	649.0
Al_2S_3 (S)	590.5	489.6	557.8	565.0	584.3	586.9	583.3	583.4
$AlCl_3$ (Al)	398.0	328.5	398.9	393.0	394.2	394.9	384.5	400.3
$AlCl_3$ (Cl)	877.4	854.0	860.2	864.6	869.5	871.8	881.8	874.4
AlF_3	492.9	447.4	489.2	489.4	488.8	489.1	484.5	493.1
AlH_3	254.7	197.6	252.3	252.4	251.3	252.1	241.3	256.8
Ar_2	1236.4	1228.9	1231.8	1231.2	1231.1	1232.9	1242.4	1242.2
As_4S_4	721.6	794.7	733.5	717.5	717.2	716.9	769.2	731.4
$AsCl_3$	480.0	437.8	463.2	481.0	474.8	476.4	511.7	496.3
BeS	1073.2	1081.5	1062.8	1059.5	1066.3	1068.1	1085.8	1074.5
BrCl	692.0	656.1	685.5	694.4	681.9	683.8	689.7	698.1
$CaCl_2$	794.2	972.5	757.4	771.1	785.4	786.6	805.3	795.7
Cl_2	417.8	347.0	384.2	412.8	413.2	414.0	414.9	424.7
ClF	−846.1	−417.7	−725.7	−789.7	−843.2	−847.5	−672.0	−819.6
ClF_3	−955.9	−735.9	−887.1	−920.0	−958.4	−958.8	−825.5	−944.5
CS_2	472.0	494.5	464.6	469.6	467.6	468.0	513.5	475.3
Cu_2S	1123.3	1654.9	1208.9	1129.8	1117.5	1115.4	1150.8	1118.8
CuCl	920.8	1284.3	1011.8	920.4	911.7	912.5	960.2	924.0
GaCl	436.0	387.0	395.4	426.8	427.8	431.9	386.0	424.7
$GaCl_3$	740.8	708.4	728.9	734.7	735.6	737.6	739.0	742.9
$GeCl_4$	565.9	508.9	555.9	566.1	564.6	565.1	582.9	573.3
H_2SO_4	117.8	114.3	140.1	119.9	110.3	110.9	125.6	121.2
H_3PO_4	260.7	240.8	272.0	259.2	254.7	255.2	256.9	256.6
HCl	926.5	915.8	917.4	917.5	919.3	921.1	936.9	921.4
HCP	323.2	316.3	316.3	315.3	318.8	320.1	292.0	318.3
H_2S	690.7	703.1	683.1	682.0	684.5	686.3	704.5	682.8
H_2S_2	525.7	520.6	517.9	515.4	519.4	521.1	545.2	519.3
K_2S	744.7	1031.0	815.5	733.2	727.5	718.8	854.3	784.4
K_3P	386.0	564.8	504.4	418.5	412.3	395.0	383.7	416.0
KCl	1006.6	1038.4	942.4	952.6	968.9	974.1	1027.2	996.0
Li_4Cl_4	995.2	1075.2	1007.6	989.0	987.4	989.1	1037.1	1022.5
LiCl	1017.9	965.7	977.7	994.1	1007.0	1011.3	972.5	1002.7
Li_2S	864.5	905.9	860.7	858.2	857.0	858.3	958.3	901.0
$MgCl_2$	1062.7	1088.1	1056.0	1044.0	1053.1	1056.6	1030.9	1052.2
Na_2S	1116.0	1153.2	1105.8	1092.4	1106.6	1109.8	1077.3	1087.1
Na_3P	1031.3	1546.4	1190.8	1025.5	1031.5	1026.8	1076.7	1039.9
NaCl	561.0	700.9	631.3	545.0	558.6	559.3	553.4	557.7
P_2	−337.5	−432.6	−349.0	−361.6	−346.5	−339.6	−380.5	−358.6
PF_3	135.8	87.6	132.8	131.2	130.2	131.4	116.7	129.8
PF_5	324.0	254.2	325.2	321.2	317.6	318.9	311.8	319.3
PH_3	567.8	601.4	567.0	562.6	562.6	563.5	553.7	562.7
Li_3P	520.1	494.4	508.0	516.4	516.3	515.6	643.4	542.3
S_5	5.8	−32.9	−4.9	9.0	2.0	2.4	44.8	12.1
S_5	−86.3	−175.9	−114.5	−91.2	−91.6	−89.2	−73.1	−85.7
S_5	−181.5	−298.2	−205.1	−186.9	−185.9	−184.0	−140.4	−173.1
$ScCl_3$	314.5	227.4	226.5	288.5	309.4	311.9	269.8	298.4
SF_2	−1172.5	−861.7	−1083.6	−1129.7	−1168.5	−1172.7	−979.7	−1156.6
SF_4	−105.7	−182.9	−110.5	−109.9	−112.4	−110.6	−63.2	−106.2
SF_6	206.7	96.9	216.9	206.3	198.7	200.1	243.6	208.2

$SiCl_4$ (Si)	311.9	219.9	309.4	307.0	307.1	307.8	298.5	309.4
$SiCl_4$ (Cl)	684.5	681.4	680.4	684.6	678.3	679.3	718.5	690.7
SiF_4	429.8	382.2	431.3	426.8	424.5	425.1	421.4	427.5
SiH_4	432.7	480.2	440.4	432.0	428.1	428.4	432.3	430.6
SiO_2	326.0	293.9	331.2	322.7	322.1	322.6	317.6	324.1
SiS_2 (Si)	192.6	131.5	198.3	188.8	188.7	189.8	182.2	190.0
SiS_2 (S)	565.7	400.2	529.5	535.7	559.1	562.3	558.8	561.4
$TiCl_4$	39.9	−38.3	−39.4	20.1	35.9	38.1	−10.6	28.1
TiS_2	−891.9	−898.4	−969.0	−907.9	−891.2	−890.7	−872.1	−905.4
$ZnCl_2$	947.4	1017.2	969.7	945.5	943.9	943.5	971.5	946.1

4.6 Group 4s

Table 38 NMR isotropic shielding constants of various molecules containing 4s elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
Ca_4	1309.1	1409.8	1308.7	1298.6	1291.6	1288.4	1364.1	1356.3
$CaCl_2$	989.9	1085.3	975.1	968.5	972.1	972.3	1050.8	1015.5
CaF_2	1100.8	1148.3	1076.3	1081.4	1085.1	1084.7	1146.7	1114.9
CaH_2	824.9	891.2	804.8	814.2	810.2	809.1	839.6	854.4
K_2	1292.8	1287.7	1279.2	1280.9	1280.9	1281.8	1290.9	1290.7
K_2S	1262.9	1263.9	1240.0	1239.3	1239.8	1240.7	1280.3	1262.0
K_3P	1265.5	1275.6	1246.9	1245.6	1245.8	1246.5	1271.8	1263.0
KBr	1253.2	1241.9	1233.6	1234.9	1234.4	1235.1	1274.9	1252.7
KCl	1257.9	1248.7	1238.5	1238.8	1238.7	1239.5	1285.1	1259.4
KF	1289.0	1282.9	1271.1	1269.2	1268.2	1268.7	1311.6	1290.8
KH	1247.3	1237.1	1225.9	1229.7	1230.0	1230.8	1245.5	1246.9

4.7 Group 3d

Table 39 NMR isotropic shielding constants of various molecules containing 3d elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
$Cr(CO)_6$	−547.2	−354.7	−549.4	−556.5	−556.1	−563.1	−495.2	−513.5
CrO_3	−3477.8	−3255.2	−3469.4	−3479.2	−3477.8	−3491.1	−3220.2	−3414.8
Cu_2	2130.3	−1511.3	2004.7	2084.0	2099.6	2106.5	2182.7	2145.4
Cu_2	−753.0	−3826.4	−1134.0	−852.8	−799.1	−762.4	−230.0	−655.2
Cu_2S	518.8	−2481.4	235.5	459.3	480.8	501.0	793.3	570.5
CuCl	1141.0	−2831.1	827.9	1071.2	1100.9	1121.9	1320.3	1183.1
CuCN	1222.8	−262.6	1079.9	1172.0	1185.9	1198.3	1390.3	1241.9
CuF	−37.0	−4772.0	−557.1	−165.2	−88.1	−41.5	363.1	41.9
CuH	1444.0	−1199.9	1153.2	1355.9	1397.0	1419.0	1607.9	1472.7
$Fe(CO)_5$	−1859.1	−1624.8	−1824.8	−1864.5	−1869.4	−1877.4	−1688.4	−1818.9
Ferrocene	−2485.8	−2406.5	−2492.1	−2496.6	−2491.2	−2505.0	−2346.8	−2447.2
$Ni(CO)_4$	−1636.6	−1429.0	−1465.0	−1632.6	−1656.9	−1658.8	−1393.8	−1594.2
$ScCl_3$	175.2	164.9	116.6	150.8	169.1	166.5	231.0	180.1
ScF_3	633.9	606.7	594.2	618.3	624.9	624.0	665.2	636.8
ScH_3	−450.2	−443.3	−510.9	−461.1	−453.3	−457.7	−426.5	−438.6
$TiCl_4$	−1000.5	−939.6	−1041.4	−1017.6	−1001.5	−1010.0	−898.1	−983.4
$Ti(CO)_4$	−6517.4	−6031.6	−6441.6	−6492.0	−6497.9	−6531.0	−6095.8	−6479.2
TiF_4	−72.0	−82.2	−127.4	−90.2	−80.0	−83.0	−45.0	−64.7
TiH_4	−2806.3	−2699.7	−2896.8	−2806.6	−2798.6	−2814.1	−2730.7	−2774.1
TiO_2	−356.3	−323.8	−388.4	−375.1	−363.1	−370.2	−296.5	−338.0
TiS_2	−1813.6	−1704.3	−1858.6	−1831.6	−1811.1	−1824.8	−1689.6	−1786.0
VH_5	−5304.3	−4951.7	−5349.6	−5293.9	−5290.1	−5314.5	−5071.1	−5234.3
Zn_2	2457.3	2431.8	2421.6	2419.2	2418.6	2423.3	2459.4	2452.3
$ZnCl_2$	1634.7	1751.6	1644.0	1614.8	1598.1	1602.1	1753.7	1632.8
ZnF_2	1644.0	1574.8	1635.8	1617.9	1606.1	1612.2	1756.8	1641.0
ZnH_2	1577.9	1733.6	1604.5	1565.9	1549.0	1550.0	1712.9	1573.8
$Zn(CH_3)_2$	1345.3	1522.2	1370.7	1333.1	1312.1	1315.8	1493.8	1338.7

4.8 Group 4p

Table 40 NMR isotropic shielding constants of various molecules containing 4p elements.

n_g	ET	pcSseg-0	pcSseg-1	pcSseg-2	pcSseg-3	pcSseg-4	SVPall-s	x2c-TZVPall-s
As_4	2248.8	2287.9	2222.2	2205.1	2203.1	2210.2	2246.1	2255.1
As_4S_4	1380.5	1402.0	1368.8	1333.7	1332.2	1342.4	1457.1	1400.4
$AsCl_3$	456.3	469.3	393.1	414.3	415.4	424.6	448.6	458.5
AsH_3	1871.9	1926.2	1832.2	1831.5	1828.8	1835.4	1869.4	1872.4
Br_2	1441.8	1293.5	1337.0	1403.1	1398.5	1407.7	1347.1	1450.9
BrCl	776.1	579.7	616.0	727.5	751.2	756.2	714.8	802.1
GaCl	1671.6	1766.5	1623.0	1627.0	1629.0	1635.5	1679.9	1673.3
$GaCl_3$	1348.2	1570.6	1305.8	1312.7	1310.8	1315.5	1416.9	1376.2
GaF	1941.3	1924.6	1882.6	1892.6	1898.8	1905.2	1937.3	1943.1
GaH_3	1045.9	1247.6	1004.6	1010.9	1008.8	1015.4	1095.1	1065.6
$GeCl_4$	1143.4	1303.9	1080.4	1105.5	1104.7	1110.3	1186.7	1177.9
GeF_4	1418.3	1525.0	1369.3	1378.4	1378.4	1385.2	1455.4	1454.4
GeH_4	1614.8	1806.3	1582.4	1577.2	1576.7	1581.4	1639.5	1635.4
GeO	901.7	971.4	883.9	845.2	861.1	867.7	980.9	898.7
GeO_2	1374.8	1463.0	1338.1	1332.9	1333.2	1339.7	1440.1	1393.3
HBr	2547.1	2424.7	2480.2	2490.6	2495.3	2504.7	2506.5	2536.8
$CHBr_3$	1256.1	1297.0	1226.8	1233.4	1220.6	1224.9	1315.6	1292.3
KBr	2907.3	2941.8	2764.4	2771.3	2792.3	2809.3	2968.2	2894.7
Kr_2	3289.3	3189.8	3217.6	3218.4	3223.0	3237.6	3291.0	3286.8
Se_8	822.4	884.8	824.9	805.0	787.1	789.6	844.9	869.3
SeH_2	2046.2	1982.1	1981.1	1996.5	2001.0	2008.3	1998.8	2037.6
SeO_2	−467.2	−357.3	−449.3	−519.2	−502.2	−498.8	−413.2	−453.3

5 Exponents and contractions coefficients of the x2c-SVPall-s and x2c-TZVPall-s basis set

The exponents and the contraction coefficients of the x2c-SVPall-s and x2c-TZVPall-s basis sets are provided in two separate text files, x2c-SVPall-s.txt and x2c-TZVPall-s.txt, as part of the supplementary material. Moreover, the derived x2c-SV(P)all-s and x2c-TZVPPall-s sets are given. These are constructed by using the polarization functions of Ref. 1.

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