Supplementary Material

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1 Hydrogen Pseudopotential and Basis Sets

A significantly improved hydrogen pseudopotential developed by Filippi and Dolg is provided in Table 1. The s contraction for the hydrogen basis sets is given in Table 2. The Gauss-Slater (GS) primitives for the double-zeta ($2z$) atomic natural orbital GS (ANO-GS) basis for hydrogen are provided in Table 3. The GS primitives for the triple-zeta ($3z$) ANO-GS basis for hydrogen are provided in Table 4. The Gaussian primitives for the quintuple-zeta ($5z$) Gaussian basis for hydrogen are provided in Table 5. Each basis was constructed using the methods of Ref. [1].

Table 1: Significantly improved pseudopotential for hydrogen developed by Filippi and Dolg to replace pseudopotential from Ref. [2, 3]. Format is appropriate for GAMESS [4].

H-QMC GEN 0 1		
3		
1.00000000	1	10.
10.	3	9.872559446615
-7.556924974646	2	10.258560602196

Table 2: s contraction for hydrogen basis sets. The contraction was constructed using the method of Ref. [1].

Exponent	Coefficient
0.05559917	0.070858475
0.11675826	0.283134279
0.24519235	0.347654627
0.51490394	0.233232914
1.08129828	0.119346810
2.27072639	0.053366645
4.76852541	0.022054957
10.01390336	0.011743843
21.02919706	0.000820785

Table 3: Primitives for $2z$ ANO-GS basis for hydrogen. The primitives were constructed using the method of Ref. [1].

Function	Exp.
GS-1S	1.946875
GS-2P	1.968750

Table 4: Primitives for $3z$ ANO-GS basis for hydrogen. The primitives were constructed using the method of Ref. [1].

Function	Exp.
GS-1S	0.925000
GS-1S	1.968750
GS-2P	1.887500
GS-2P	2.553125
GS-3D	2.659375

Table 5: Primitives for $5z$ Gaussian basis for hydrogen. The primitives were constructed using the method of Ref. [1].

Function	Exp.
1S	0.0692135
1S	0.1736131
1S	0.4543641
1S	1.3072524
2P	0.2370069
2P	0.6258464
2P	1.6114234
2P	5.1965679
3D	0.5106775
3D	1.3660613
3D	3.2652161
4F	0.6792030
4F	2.0042817

2   Setup and Reference Data

The geometries, zero point energies, and experimental atomization energies for the molecules of the G2 set [5] are provided in Table 6.

Table 6: Geometries, zero point energies, and experimental atomization energies for the molecules of the G2 set [5]. Some experimental error bars were not available (N/A).

System	Geometry	ZPE (kcal/mol)	Expt. Atomization Energy (kcal/mol)
LiH	[6]	1.99 [6]	56 ± 0.01 [7]
BeH	[6]	2.92 [6]	46.9 ± 0.01 [7]
CH	[6]	4.04 [6]	79.9 ± 0.02 [7]
CH_2 $(^3B_1)$	[6]	10.55 [6]	179.6 ± N/A [7]
CH_2 $(^1A_1)$	[6]	10.29 [6]	170.6 ± N/A [7]
CH_3	[6]	18.55 [6]	289.3 ± 0.2 [7]
CH_4	[6]	27.74 [6]	392.5 ± 0.1 [7]
NH	[6]	4.64 [6]	79 ± 0.4 [7]
NH_2	[6]	11.84 [6]	170 ± 0.3 [7]
NH_3	[6]	21.33 [6]	276.7 ± 0.1 [7]
OH	[6]	5.29 [6]	101.4 ± 0.3 [7]
H_2O	[6]	13.26 [6]	219.35 ± 0.01 [7]
HF	[6]	5.86 [6]	135.2 ± 0.2 [7]
SiH_2 $(^1A_1)$	[8]	7.3 [7]	144.4 ± 0.7 [7]
SiH_2 $(^3B_1)$	[9]	7.5 [7]	123.4 ± 0.7 [7]
SiH_3	[8]	13.2 [7]	213.8 ± 1.2 [7]
SiH_4	[8]	19.4 [7]	302.6 ± 0.5 [7]
PH_2	[8]	8.4 [7]	144.7 ± 0.6 [7]
PH_3	[6]	14.44 [6]	228.6 ± 0.4 [7]
H_2S	[6]	9.4 [6]	173.1 ± 0.2 [7]
HCl	[6]	4.24 [6]	102.24 ± 0.5 [7]
Li_2	[10]	0.5 [6]	23.9 ± 0.7 [7]
LiF	[10]	1.3 [7]	137.6 ± 2 [7]
C_2H_2	[6]	16.5 [6]	386.9 ± 0.2 [7]
C_2H_4	[6]	31.66 [6]	531.9 ± 0.1 [7]
C_2H_6	[6]	46.23 [6]	666.3 ± N/A [7]
CN	[6]	2.95 [6]	178.1 ± 2.4 [7]
HCN	[6]	9.95 [6]	301.7 ± 2 [7]
CO	[6]	3.09 [6]	256.2 ± 0.2 [7]
HCO	[6]	8.09 [6]	270.3 ± 2 [7]
H_2CO	[6]	16.52 [6]	357.2 ± 0.1 [7]
H_3COH	[8]	31.72 [6]	480.8 ± N/A [7]
N_2	[6]	3.36 [6]	225.1 ± 0.4 [7]
N_2H_4	[8]	32.68 [6]	405.4 ± N/A [7]
NO	[6]	2.71 [6]	150.06 ± 0.04 [7]
O_2	[10]	2.25 [6]	117.96 ± 0.02 [7]
H_2O_2	[6]	16.44 [6]	252.3 ± N/A [7]
F_2	[10]	1.3 [6]	36.9 ± 0.1 [7]
CO_2	[6]	7.24 [6]	381.93 ± 0.01 [7]
Na_2	[8]	0.2 [7]	16.8 ± 0.3 [7]
Si_2	[10]	0.73 [6]	74 ± N/A [7]
P_2	[10]	1.11 [6]	116.1 ± 0.5 [7]

Table 6 – continued

System	Geometry	ZPE (kcal/mol)	Expt. Atomization Energy (kcal/mol)
S_2	[10]	1.04 [6]	100.66 ± 0.07 [7]
Cl_2	[6]	0.8 [6]	57.18 ± 0.01 [7]
NaCl	[8]	0.5 [7]	97.3 ± 0.5 [7]
SiO	[6]	1.78 [6]	189.9 ± 2 [7]
CS	[10]	1.83 [6]	169.4 ± 6 [7]
SO	[6]	1.63 [6]	123.4 ± 0.3 [7]
ClO	[10]	1.22 [6]	63.42 ± 0.02 [7]
ClF	[6]	1.12 [6]	$60.4 \pm N/A$ [7]
Si_2H_6	[8]	30.5 [7]	$500.1 \pm N/A$ [7]
CH_3Cl	[6]	23.19 [6]	$371 \pm N/A$ [7]
H_3CSH	[8]	28.6 [7]	$445.1 \pm N/A$ [7]
HOCl	[6]	8.18 [6]	156.3 ± 0.5 [7]
SO_2	[10]	4.38 [6]	254 ± 0.2 [7]

3 Raw Data

3.1 Locality Approximation

This section contains the raw data for those systems handled with the locality approximation [11]. The diffusion Monte Carlo (DMC) total energies of the molecules from the G2 set and their atoms for a single determinant Slater-Jastrow (SJ) trial wavefunction composed of Hartree-Fock (HF) orbitals are given in Table 7. The DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of variational Monte Carlo (VMC) optimized orbitals are given in Table 8. The DMC total energies of the molecules from the G2 set and their atoms for a CAS SJ trial wavefunction with an s and p active space are given in Table 9. The DMC total energies of the phosphorus containing molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of VMC optimized orbitals, a CAS SJ trial wavefunction with an s and p active space, and a CAS SJ trial wavefunction with an s, p, and d active space are given in Table 10.

Table 7: DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of HF orbitals. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	$2z$	$3z$	$5z$
H	-0.5000006(1)	-0.5000006(1)	-0.5000006(1)
Li	-0.1963297(5)	-0.1963297(7)	-0.196329(2)
C	-5.42251(7)	-5.42233(8)	-5.42236(7)
N	-9.79127(7)	-9.79109(5)	-9.79123(6)
O	-15.89289(8)	-15.89228(8)	-15.89254(8)
F	-24.18633(8)	-24.18594(7)	-24.18609(7)
Na	-0.1821457(7)	-0.1821441(7)	-0.182145(2)
Si	-3.76661(5)	-3.76662(5)	-3.76654(5)
P	-6.47660(7)	-6.47648(5)	-6.47645(7)
S	-10.13125(9)	-10.13103(9)	-10.1311(1)
Cl	-14.97223(6)	-14.97168(6)	-14.97179(6)
CH	-6.05266(7)	-6.05399(9)	-6.05422(8)
CH_2 ($^1A_1$)	-6.7061(1)	-6.70751(9)	-6.70792(9)
CH_3	-7.41421(9)	-7.41476(8)	-7.41490(8)

Table 7 – continued

System	2z	3z	5z
CH$_4$	-8.09421(9)	-8.09441(9)	-8.09451(8)
NH	-10.41946(8)	-10.42028(7)	-10.42068(8)
NH$_2$	-11.07601(9)	-11.07774(9)	-11.07834(9)
NH$_3$	-11.7593(1)	-11.76181(8)	-11.76266(9)
OH	-16.56031(9)	-16.56126(9)	-16.56142(9)
H$_2$O	-17.25949(8)	-17.26123(8)	-17.26175(9)
HF	-24.90895(8)	-24.91024(7)	-24.91083(8)
SiH$_2$ (^{1}A$_1$)	-5.00856(7)	-5.00925(7)	-5.00952(7)
SiH$_2$ (^{3}B$_1$)	-4.97656(7)	-4.97723(7)	-4.97709(6)
SiH$_3$	-5.6280(1)	-5.62910(8)	-5.62906(9)
SiH$_4$	-6.28261(9)	-6.28418(8)	-6.28428(7)
PH$_2$	-7.71744(8)	-7.71798(8)	-7.71812(8)
PH$_3$	-8.35619(7)	-8.35676(7)	-8.35696(7)
H$_2$S	-11.41932(8)	-11.41962(7)	-11.42012(7)
HCl	-15.64183(8)	-15.64178(8)	-15.64211(8)
Li$_2$	-0.43045(2)	-0.43053(3)	-0.43053(2)
C$_2$H$_4$	-13.74229(8)	-13.7433(1)	-13.74348(8)
C$_2$H$_6$	-14.98415(8)	-14.9851(1)	-14.9850(1)
CO	-21.7192(1)	-21.7232(1)	-21.7238(1)
H$_2$CO	-22.9038(1)	-22.9080(1)	-22.9082(1)
H$_3$COH	-24.12892(9)	-24.13207(8)	-24.13271(8)
N$_2$	-19.9296(1)	-19.9333(1)	-19.9338(1)
N$_2$H$_4$	-22.26561(9)	-22.27033(9)	-22.27206(8)
NO	-25.9062(1)	-25.9108(1)	-25.9117(1)
O$_2$	-31.9642(1)	-31.9679(1)	-31.9691(1)
H$_2$O$_2$	-33.1973(1)	-33.2013(1)	-33.2025(1)
F$_2$	-48.4134(1)	-48.4146(1)	-48.41757(9)
CO$_2$	-37.8168(1)	-37.8228(1)	-37.8235(1)
Na$_2$	-0.39102(2)	-0.39106(2)	-0.39104(2)
Si$_2$	-7.6498(1)	-7.6505(1)	-7.65031(9)
P$_2$	-13.1256(1)	-13.1273(1)	-13.1275(1)
S$_2$	-20.4191(1)	-20.4207(1)	-20.4214(1)
Cl$_2$	-30.0309(1)	-30.0305(1)	-30.03165(9)
SiO	-19.9535(1)	-19.96031(9)	-19.96104(8)
CS	-15.8151(1)	-15.8169(1)	-15.8185(1)
SO	-26.2105(1)	-26.2159(1)	-26.21669(9)
ClO	-30.9457(1)	-30.9475(1)	-30.9486(1)
ClF	-39.2434(1)	-39.24608(9)	-39.2478(1)
Si$_2$H$_6$	-11.3836(1)	-11.3857(1)	-11.38579(9)
CH$_3$Cl	-22.5236(1)	-22.5245(1)	-22.5249(1)
H$_3$CSH	-18.30598(9)	-18.3071(1)	-18.30752(9)
HOCl	-31.61547(9)	-31.6179(1)	-31.6193(1)
SO$_2$	-42.2986(1)	-42.3125(1)	-42.3152(1)

Table 8: The DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of VMC optimized orbitals. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	$2z$	$3z$	$5z$
H	-0.5000005(1)	-0.5000006(1)	-0.5000005(1)
Li	-0.1963295(4)	-0.1963292(4)	-0.1963296(3)
C	-5.42288(7)	-5.42292(7)	-5.42296(6)
N	-9.79213(6)	-9.79230(6)	-9.79229(6)
O	-15.8930(1)	-15.89305(8)	-15.89310(7)
F	-24.18619(5)	-24.18651(7)	-24.18636(8)
Na	-0.1821438(7)	-0.1821446(4)	-0.1821438(4)
Si	-3.76682(5)	-3.76676(4)	-3.76683(4)
P	-6.47688(9)	-6.47699(5)	-6.47686(5)
S	-10.1317(1)	-10.13184(8)	-10.13189(7)
Cl	-14.97253(6)	-14.97252(6)	-14.97261(6)
CH	-6.05388(8)	-6.05473(7)	-6.05476(9)
CH_2 ($^1A_1$)	-6.70711(9)	-6.70861(8)	-6.70860(7)
CH_3	-7.41489(7)	-7.41544(9)	-7.41549(7)
CH_4	-8.09523(7)	-8.09523(8)	-8.09523(8)
NH	-10.42146(8)	-10.42200(8)	-10.42186(7)
NH_2	-11.07824(9)	-11.07960(8)	-11.07962(8)
NH_3	-11.76205(8)	-11.76368(7)	-11.76378(7)
OH	-16.56188(9)	-16.56243(8)	-16.56264(9)
H_2O	-17.26195(8)	-17.26298(8)	-17.26313(8)
HF	-24.91098(7)	-24.91170(6)	-24.91175(7)
SiH_2 ($^1A_1$)	-5.00947(5)	-5.01034(5)	-5.01055(4)
SiH_2 ($^3B_1$)	-4.97846(4)	-4.97932(3)	-4.97952(3)
SiH_3	-5.62975(6)	-5.63077(6)	-5.63097(5)
SiH_4	-6.28405(6)	-6.28526(5)	-6.28548(5)
PH_2	-7.71870(8)	-7.71952(6)	-7.71994(6)
PH_3	-8.35790(7)	-8.35892(5)	-8.35921(6)
H_2S	-11.42111(8)	-11.42203(7)	-11.42238(7)
HCl	-15.64294(7)	-15.64345(7)	-15.64374(7)
Li_2	-0.43069(2)	-0.43069(5)	-0.43077(4)
C_2H_4	-13.74413(7)	-13.74453(6)	-13.74477(7)
C_2H_6	-14.98622(7)	-14.98643(7)	-14.98640(6)
CO	-21.72262(9)	-21.72572(9)	-21.72617(9)
H_2CO	-22.9080(1)	-22.91048(9)	-22.91083(9)
H_3COH	-24.13189(8)	-24.13417(7)	-24.1348(1)
N_2	-19.93256(9)	-19.93600(9)	-19.93638(9)
N_2H_4	-22.26927(9)	-22.27373(7)	-22.27469(8)
NO	-25.9119(1)	-25.91612(9)	-25.91693(9)
O_2	-31.9682(1)	-31.9707(1)	-31.9719(1)
H_2O_2	-33.2030(1)	-33.20627(8)	-33.20778(9)
F_2	-48.4216(1)	-48.42302(9)	-48.42522(8)
CO_2	-37.8259(1)	-37.8287(1)	-37.8291(1)
Na_2	-0.39104(1)	-0.39104(4)	-0.39106(2)
Si_2	-7.65138(6)	-7.65274(8)	-7.65279(7)
P_2	-13.12785(9)	-13.1300(1)	-13.13077(9)
S_2	-20.4211(1)	-20.4236(1)	-20.4248(1)

Table 8 – continued

System	$2z$	$3z$	$5z$
Cl_2	-30.03397(9)	-30.03514(9)	-30.03684(8)
SiO	-19.95896(9)	-19.96336(9)	-19.96385(7)
CS	-15.81932(9)	-15.82302(9)	-15.82387(8)
SO	-26.21600(9)	-26.22047(9)	-26.22172(9)
ClO	-30.9600(1)	-30.96312(9)	-30.96463(9)
ClF	-39.24935(9)	-39.25234(7)	-39.25406(8)
Si_2H_6	-11.38585(8)	-11.38818(7)	-11.38840(7)
CH_3Cl	-22.5259(1)	-22.5266(1)	-22.5275(1)
H_3CSH	-18.30852(9)	-18.30988(8)	-18.31105(7)
HOCl	-31.62113(9)	-31.62387(9)	-31.62501(8)
SO_2	-42.3125(1)	-42.32256(8)	-42.32431(8)

Table 9: The DMC total energies of the molecules from the G2 set and their atoms for a CAS SJ trial wavefunction with an s and p active space. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	$3z$
H	-0.5000006(1)
Li	-0.1963292(4)
C	-5.42823(6)
N	-9.79230(6)
O	-15.89305(8)
F	-24.18651(7)
Na	-0.1821446(4)
Si	-3.76711(4)
P	-6.47699(5)
S	-10.13184(8)
Cl	-14.97252(6)
CH	-6.06239(6)
CH_2 ($^1A_1$)	-6.71713(6)
CH_3	-7.41764(6)
CH_4	-8.09730(6)
NH	-10.42390(7)
NH_2	-11.08219(7)
NH_3	-11.76623(6)
OH	-16.56411(8)
H_2O	-17.26521(7)
HF	-24.91286(7)
SiH_2 ($^1A_1$)	-5.01238(4)
SiH_2 ($^3B_1$)	-4.97970(3)
SiH_3	-5.63114(4)
SiH_4	-6.28571(4)
PH_2	-7.72051(5)
PH_3	-8.36003(5)
H_2S	-11.42305(7)
HCl	-15.64382(5)
Li_2	-0.431584(5)
C_2H_4	-13.75239(8)

Table 9 – continued

System	$3z$
C_2H_6	-14.99037(9)
CO	-21.73788(7)
H_2CO	-22.9190(1)
H_3COH	-24.14011(5)
N_2	-19.95032(7)
N_2H_4	-22.27934(5)
NO	-25.92787(8)
O_2	-31.97692(9)
H_2O_2	-33.21410(9)
F_2	-48.43320(8)
CO_2	-37.83890(7)
Na_2	-0.39106(2)
Si_2	-7.65485(7)
P_2	-13.13441(8)
S_2	-20.42452(9)
Cl_2	-30.03679(9)
SiO	-19.96885(7)
CS	-15.83223(6)
SO	-26.22235(9)
ClO	-30.96605(8)
ClF	-39.25596(7)
Si_2H_6	-11.38838(7)
CH_3Cl	-22.52839(7)
H_3CSH	-18.3128(1)
HOCl	-31.6278(1)
SO_2	-42.33049(6)

Table 10: The DMC total energies of the phosphorus containing molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of VMC optimized orbitals, a CAS SJ trial wavefunction with an s and p active space, and a CAS SJ trial wavefunction with an s, p, and d active space. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	1CSF	s, p CAS	s, p, d CAS
H	-0.5000006(1)	-0.5000006(1)	-0.5000006(1)
P	-6.47699(5)	-6.47699(5)	-6.47753(5)
PH_2	-7.71952(6)	-7.72051(5)	-7.72183(5)
PH_3	-8.35892(5)	-8.36003(5)	-8.36145(6)
P_2	-13.1300(1)	-13.13441(8)	-13.13814(7)

3.2   T-Moves

This section contains the raw data for those systems handled with the size-consistent version of T-Moves [12]. The DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of HF orbitals are given in Table 11. The DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of VMC optimized

orbitals are given in Table 12. The DMC total energies of the molecules from the G2 set and their atoms for a CAS SJ trial wavefunction with an s and p active space are given in Table 13.

Table 11: DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of HF orbitals. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	$2z$	$3z$	$5z$
H	-0.5000006(1)	-0.5000006(1)	-0.5000006(1)
Li	-0.1963297(5)	-0.1963297(7)	-0.196329(2)
Be	-1.00918(5)	-1.00928(4)	-1.00926(5)
C	-5.42211(7)	-5.42206(7)	-5.42194(6)
N	-9.79121(5)	-9.79092(6)	-9.79123(6)
O	-15.89194(8)	-15.89176(8)	-15.89184(7)
F	-24.18514(7)	-24.18515(7)	-24.18527(7)
Na	-0.1821457(7)	-0.1821441(7)	-0.182145(2)
Cl	-14.97154(6)	-14.97117(6)	-14.97115(7)
LiH	-0.78787(3)	-0.78800(2)	-0.78799(1)
BeH	-1.58814(6)	-1.58861(4)	-1.58849(5)
CH_2 ($^3B_1$)	-6.72719(9)	-6.72762(7)	-6.72777(8)
LiF	-24.60333(8)	-24.60401(8)	-24.60477(7)
C_2H_2	-12.4878(1)	-12.48906(9)	-12.48920(7)
CN	-15.48083(8)	-15.4833(1)	-15.48371(8)
HCN	-16.20259(8)	-16.20468(8)	-16.20494(9)
HCO	-22.24632(9)	-22.25065(8)	-22.25173(9)
NaCl	-15.31021(6)	-15.31104(8)	-15.31135(7)

Table 12: The DMC total energies of the molecules from the G2 set and their atoms for a single determinant SJ trial wavefunction composed of VMC optimized orbitals. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	$2z$	$3z$	$5z$
H	-0.5000005(1)	-0.5000006(1)	-0.5000005(1)
Li	-0.1963295(4)	-0.1963292(4)	-0.1963296(3)
Be	-1.00921(5)	-1.00916(5)	-1.00924(4)
C	-5.42244(6)	-5.42258(5)	-5.42245(5)
N	-9.79214(6)	-9.79210(6)	-9.79218(6)
O	-15.89241(9)	-15.89249(7)	-15.89272(7)
F	-24.18526(5)	-24.18535(7)	-24.18548(7)
Na	-0.1821438(7)	-0.1821446(4)	-0.1821438(4)
Cl	-14.97209(6)	-14.97204(6)	-14.97212(5)
LiH	-0.78804(1)	-0.78804(1)	-0.788051(9)
BeH	-1.58833(4)	-1.58887(3)	-1.58883(3)
CH_2 ($^3B_1$)	-6.72867(7)	-6.72921(7)	-6.72940(6)
LiF	-24.60451(8)	-24.60473(8)	-24.60479(8)
C_2H_2	-12.4900(1)	-12.49043(7)	-12.49048(8)
CN	-15.49091(9)	-15.49296(8)	-15.49339(8)
HCN	-16.20593(8)	-16.20711(7)	-16.20741(7)
HCO	-22.25183(8)	-22.25561(6)	-22.25607(7)

Table 12 – continued

System	$2z$	$3z$	$5z$
NaCl	-15.31167(5)	-15.31196(6)	-15.31202(7)

Table 13: The DMC total energies of the molecules from the G2 set and their atoms for a CAS SJ trial wavefunction with an s and p active space. Energies are in Hartrees. Error bar, which is shown in parentheses, is for the last digit.

System	$3z$
H	-0.5000006(1)
Li	-0.1963292(4)
Be	-1.010186(5)
C	-5.42775(5)
N	-9.79230(6)
O	-15.89305(8)
F	-24.18651(7)
Na	-0.1821446(4)
Cl	-14.97252(6)
LiH	-0.788238(6)
BeH	-1.59014(2)
CH_2 ($^3B_1$)	-6.73142(8)
LiF	-24.61011(7)
C_2H_2	-12.50101(5)
CN	-15.50866(7)
HCN	-16.22003(6)
HCO	-22.26378(7)
NaCl	-15.31334(6)

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