

Table 1: A set of choices for the PAO basis functions from E to Kr.

VPS	Valence electrons	Quick	Standard	Precise
E	0.0	Kr10.0-s1p1	Kr10.0-s2p1d1	Kr10.0-s2p2d1f1
H_PBE19	1.0	H5.0-s2	H6.0-s2p1	H7.0-s2p2d1
He_PBE19	2.0	He8.0-s1p1	He8.0-s2p1	He10.0-s2p2d1
Li_PBE19	3.0	Li8.0-s3p1	Li8.0-s3p2	Li8.0-s3p2d1
Be_PBE19	2.0	Be7.0-s2p1	Be7.0-s2p2	Be7.0-s3p2d1
B_PBE19	3.0	B7.0-s2p2	B7.0-s2p2d1	B7.0-s3p2d2
C_PBE19	4.0	C6.0-s2p2	C6.0-s2p2d1	C6.0-s3p2d2
N_PBE19	5.0	N6.0-s2p2	N6.0-s2p2d1	N6.0-s3p2d2
O_PBE19	6.0	O6.0-s2p2	O6.0-s2p2d1	O6.0-s3p2d2
F_PBE19	7.0	F6.0-s2p2	F6.0-s2p2d1	F6.0-s3p3d2f1
Ne_PBE19	8.0	Ne9.0-s2p2	Ne9.0-s2p2d1	Ne9.0-s3p2d2
Na_PBE19	9.0	Na9.0-s3p2	Na9.0-s3p2d1	Na9.0-s3p2d2
Mg_PBE19	8.0	Mg9.0-s2p2	Mg9.0-s3p2d1	Mg9.0-s3p2d2
Al_PBE19	3.0	Al7.0-s2p1d1	Al7.0-s2p2d1	Al7.0-s3p2d2
Si_PBE19	4.0	Si7.0-s2p1d1	Si7.0-s2p2d1	Si7.0-s3p3d2
P_PBE19	5.0	P7.0-s2p2d1	P7.0-s2p2d1f1	P7.0-s3p2d2f1
S_PBE19	6.0	S7.0-s2p2d1	S7.0-s2p2d1f1	S7.0-s3p2d2f1
Cl_PBE19	7.0	Cl7.0-s2p2d1	Cl7.0-s2p2d1f1	Cl7.0-s3p2d2f1
Ar_PBE19	8.0	Ar9.0-s2p2d1	Ar9.0-s2p2d1f1	Ar9.0-s3p2d2f1
K_PBE19	9.0	K10.0-s3p2	K10.0-s3p2d1	K10.0-s3p2d2
Ca_PBE19	10.0	Ca9.0-s3p2	Ca9.0-s3p2d1	Ca9.0-s3p2d2
Sc_PBE19	11.0	Sc9.0-s2p2d1	Sc9.0-s3p2d1	Sc9.0-s3p2d2
Ti_PBE19	12.0	Ti7.0-s2p2d1	Ti7.0-s3p2d1	Ti7.0-s3p2d2f1
V_PBE19	13.0	V6.0-s2p2d1	V6.0-s3p2d1	V6.0-s3p2d2f1
Cr_PBE19	14.0	Cr6.0-s2p2d1	Cr6.0-s3p2d1	Cr6.0-s3p2d2f1
Mn_PBE19	15.0	Mn6.0-s2p2d1	Mn6.0-s3p2d1	Mn6.0-s3p2d2f1
Fe_PBE19H	16.0	Fe5.5H-s2p2d1	Fe5.5H-s3p2d1	Fe5.5H-s3p2d2f1
Fe_PBE19S	14.0	Fe6.0S-s2p2d1	Fe6.0S-s3p2d1	Fe6.0S-s3p2d2f1
Co_PBE19H	17.0	Co6.0H-s2p2d1	Co6.0H-s3p2d1	Co6.0H-s3p2d2f1
Co_PBE19S	15.0	Co6.0S-s2p2d1	Co6.0S-s3p2d1	Co6.0S-s3p2d2f1
Ni_PBE19H	18.0	Ni6.0H-s2p2d1	Ni6.0H-s3p2d1	Ni6.0H-s3p2d2f1
Ni_PBE19S	16.0	Ni6.0S-s2p2d1	Ni6.0S-s3p2d1	Ni6.0S-s3p2d2f1
Cu_PBE19H	19.0	Cu6.0H-s2p2d1	Cu6.0H-s3p2d1	Cu6.0H-s3p2d2f1
Cu_PBE19S	11.0	Cu6.0S-s2p1d1	Cu6.0S-s3p2d1	Cu6.0S-s3p2d2f1
Zn_PBE19H	20.0	Zn6.0H-s2p2d1	Zn6.0H-s3p2d1	Zn6.0H-s3p2d2f1
Zn_PBE19S	12.0	Zn6.0S-s2p1d1	Zn6.0S-s3p2d1	Zn6.0S-s3p2d2f1
Ga_PBE19	13.0	Ga7.0-s2p2d1	Ga7.0-s3p2d2	Ga7.0-s3p2d2f1
Ge_PBE19	4.0	Ge7.0-s2p1d1	Ge7.0-s3p2d2	Ge7.0-s3p2d2f1
As_PBE19	15.0	As7.0-s3p2d1	As7.0-s3p2d2	As7.0-s3p2d2f1
Se_PBE19	6.0	Se7.0-s3p2d1	Se7.0-s3p2d2	Se7.0-s3p2d2f1
Br_PBE19	7.0	Br7.0-s3p2d1	Br7.0-s3p2d2	Br7.0-s3p2d2f1
Kr_PBE19	8.0	Kr10.0-s2p2d1	Kr10.0-s3p2d2	Kr10.0-s3p2d2f1

Table 2: A set of choices for the PAO basis functions from Rb to Bi.

VPS	Valence electrons	Quick	Standard	Precise
Rb_PBE19	9.0	Rb11.0-s2p2d1	Rb11.0-s3p2d2	Rb11.0-s3p2d2f1
Sr_PBE19	10.0	Sr10.0-s2p2d1	Sr10.0-s3p2d2	Sr10.0-s3p3d2f1
Y_PBE19	11.0	Y10.0-s3p2d1	Y10.0-s3p2d2	Y10.0-s3p3d2f1
Zr_PBE19	12.0	Zr7.0-s3p2d1	Zr7.0-s3p2d2	Zr7.0-s3p2d2f1
Nb_PBE19	13.0	Nb7.0-s3p2d1	Nb7.0-s3p2d2	Nb7.0-s3p2d2f1
Mo_PBE19	14.0	Mo7.0-s3p2d1	Mo7.0-s3p2d2	Mo7.0-s3p2d2f1
Tc_PBE19	15.0	Tc7.0-s3p2d1	Tc7.0-s3p2d2	Tc7.0-s3p2d2f1
Ru_PBE19	14.0	Ru7.0-s3p2d1	Ru7.0-s3p2d2	Ru7.0-s3p2d2f1
Rh_PBE19	15.0	Rh7.0-s3p2d1	Rh7.0-s3p2d2	Rh7.0-s3p2d2f1
Pd_PBE19	16.0	Pd7.0-s3p2d1	Pd7.0-s3p2d2	Pd7.0-s3p2d2f1
Ag_PBE19	17.0	Ag7.0-s3p2d1	Ag7.0-s3p2d2	Ag7.0-s3p2d2f1
Cd_PBE19	12.0	Cd7.0-s3p2d1	Cd7.0-s3p2d2	Cd7.0-s3p2d2f1
In_PBE19	13.0	In7.0-s3p2d1	In7.0-s3p2d2	In7.0-s3p2d2f1
Sn_PBE19	14.0	Sn7.0-s3p2d1	Sn7.0-s3p2d2	Sn7.0-s3p2d2f1
Sb_PBE19	15.0	Sb7.0-s3p2d1	Sb7.0-s3p2d2	Sb7.0-s3p2d2f1
Te_PBE19	16.0	Te7.0-s3p2d2	Te7.0-s3p2d2f1	Te7.0-s3p3d2f1
I_PBE19	7.0	I7.0-s3p2d2	I7.0-s3p2d2f1	I7.0-s3p3d2f1
Xe_PBE19	8.0	Xe11.0-s3p2d1	Xe11.0-s3p2d2	Xe11.0-s3p2d2f1
Cs_PBE19	9.0	Cs12.0-s3p2d1	Cs12.0-s3p2d2	Cs12.0-s3p2d2f1
Ba_PBE19	10.0	Ba10.0-s3p2d1	Ba10.0-s3p2d2	Ba10.0-s3p2d2f1
La_PBE19	11.0	La8.0-s3p2d1f1	La8.0-s3p2d2f1	La8.0-s3p3d2f1
Ce_PBE19	12.0	Ce8.0-s3p2d1f1	Ce8.0-s3p2d2f1	Ce8.0-s3p3d2f1
Pr_PBE19	13.0	Pr8.0-s3p2d1f1	Pr8.0-s3p2d2f1	Pr8.0-s3p3d2f1
Nd_PBE19	14.0	Nd8.0-s3p2d1f1	Nd8.0-s3p2d2f1	Nd8.0-s3p3d2f1
Pm_PBE19	15.0	Pm8.0-s3p2d1f1	Pm8.0-s3p2d2f1	Pm8.0-s3p3d2f1
Sm_PBE19	16.0	Sm8.0-s3p2d1f1	Sm8.0-s3p2d2f1	Sm8.0-s3p3d2f1
Dy_PBE19	20.0	Dy8.0-s3p2d1f1	Dy8.0-s3p2d2f1	Dy8.0-s3p3d2f1
Ho_PBE19	21.0	Ho8.0-s3p2d1f1	Ho8.0-s3p2d2f1	Ho8.0-s3p3d2f1
Lu_PBE19	11.0	Lu8.0-s3p2d2	Lu8.0-s3p2d2f1	Lu8.0-s3p3d2f1
Hf_PBE19	12.0	Hf9.0-s3p2d2	Hf9.0-s3p2d2f1	Hf9.0-s3p3d2f1
Ta_PBE19	13.0	Ta7.0-s3p2d2	Ta7.0-s3p2d2f1	Ta7.0-s3p3d2f1
W_PBE19	12.0	W7.0-s3p2d2	W7.0-s3p2d2f1	W7.0-s3p3d2f1
Re_PBE19	15.0	Re7.0-s3p2d2	Re7.0-s3p2d2f1	Re7.0-s3p3d2f1
Os_PBE19	14.0	Os7.0-s3p2d2	Os7.0-s3p2d2f1	Os7.0-s3p3d2f1
Ir_PBE19	15.0	Ir7.0-s3p2d2	Ir7.0-s3p2d2f1	Ir7.0-s3p3d2f1
Pt_PBE19	16.0	Pt7.0-s3p2d2	Pt7.0-s3p2d2f1	Pt7.0-s3p3d2f1
Au_PBE19	17.0	Au7.0-s3p2d2	Au7.0-s3p2d2f1	Au7.0-s3p3d2f1
Hg_PBE19	18.0	Hg8.0-s3p2d2	Hg8.0-s3p2d2f1	Hg8.0-s3p3d2f1
Tl_PBE19	19.0	Tl8.0-s3p2d2	Tl8.0-s3p2d2f1	Tl8.0-s3p3d2f1
Pb_PBE19	14.0	Pb8.0-s3p2d2	Pb8.0-s3p2d2f1	Pb8.0-s3p3d2f1
Bi_PBE19	15.0	Bi8.0-s3p2d2	Bi8.0-s3p2d2f1	Bi8.0-s3p3d2f1