

Supporting Information Available

Table S1 Determined coefficient of a single ζ parameter in a Slater-type atomic orbital. Coefficients a_0 , a_1 , a_2 , a_3 , a_4 , and a_5 used in eq. (6).

Element	AO	a_0	a_1	a_2	a_3	a_4	a_5	$coef$
C	<i>s</i>	4.3100	0.1045	0.0195	-0.0056	-0.0012	0.0000	1.00
	<i>p</i>	1.7409	0.1440	-0.0610	0.0322	-0.0012	-0.0005	1.00
O	<i>s</i>	2.7450	0.0802	0.0185	0.0007	0.000	0.000	1.00
	<i>p</i>	2.6064	0.5181	1.0817	1.1475	0.000	0.000	1.00
H	<i>s</i>	0.9484	1.5974	0.0000	0.0000	0.000	0.000	1.00
Mg	<i>s</i>	1.7355	0.1040	0.0980	-0.1450	0.000	0.000	1.00
	<i>p</i>	1.6889	0.0673	0.0377	-0.0071	0.000	0.000	1.00
Pd	<i>s</i>	2.0000	4.4211	0.000	0.000	0.000	0.000	1.00
	<i>p</i>	1.9000	5.2163	0.0000	0.000	0.000	0.000	1.00
	<i>d</i>	2.6000	2.6810	0.0000	0.000	0.000	0.000	1.00

Table S2 Determined coefficient parameter of H_{rr} parameter. Coefficients b_0 , b_1 , b_2 , b_3 , b_4 , and b_5 used in eq. (7).

Element	AO	b_0	b_1	b_2	b_3	b_4	b_5
C	<i>S</i>	-10.6984	-11.8180	-1.4167	0.0161	0.0477	0.0106
	<i>P</i>	-8.8127	-11.7230	-1.6433	0.0032	0.0885	0.0000
O	<i>S</i>	-28.6466	-15.0328	-1.4510	-0.4949	0.0419	0.0000
	<i>P</i>	-14.6121	-14.8159	-1.6244	0.0154	0.0434	0.0010
H	<i>S</i>	-6.2010	-17.870	0.0000	0.0000	0.0000	0.0000
Mg	<i>S</i>	-7.6460	-6.2408	-0.0274	0.1793	0.0396	0.0026
	<i>P</i>	-4.9905	-6.1921	-0.0274	0.1793	0.0396	0.0026
Pd	<i>S</i>	-5.4000	-7.4547	-0.0000	0.0000	0.0000	0.0000
	<i>P</i>	-2.9000	-0.5000	-0.0000	0.0008	0.0000	0.0000
	<i>D</i>	-9.0000	-2.1314	-0.0000	0.0000	0.0000	0.0000