

ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 44 (5). THE HARTREE-FOCK FUNCTIONS FOR NEGATIVE IONS.

SULFUR K(2)L(8)3S(2)3P(5), 2P
T.E.=-0.39753820D+03 P.E.=-0.79507644D+03 K.E.= 0.39753824D+03 V.T.=-0.19999999D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-91.67593	-8.67515	-0.57932	BASIS/ORB E	-6.35496	-0.10739
1S 15.78440	0.92673	-0.25928	-0.07376	2P 7.07744	0.65158	-0.15153
1S 24.31730	0.03436	-0.00781	-0.00186	2P 12.99860	0.03916	-0.00927
2S 6.72829	0.00485	0.80034	0.24398	3P 2.62059	0.01316	0.29742
2S 14.02420	0.04839	-0.13560	-0.04061	3P 0.89975	0.00095	0.33297
3S 2.55720	0.00025	0.00504	-0.69742	3P 5.42495	0.37601	-0.10428
3S 1.48480	-0.00012	-0.00015	-0.43754	3P 1.65797	-0.00214	0.52358
3S 5.68198	-0.00131	0.35078	0.17086			

CHLORINE K(2)L(8)3S(2)3P(6), 1S
T.E.=-0.45957670D+03 P.E.=-0.91915621D+03 K.E.= 0.45957951D+03 V.T.=-0.19999939D+01

S	1S	2S	3S	P	2P	3P
BASIS/ORB E	-104.50515	-10.22891	-0.73295	BASIS/ORB E	-7.69533	-0.14992
1S 17.24050	0.92389	-0.25955	-0.07613	2P 7.62972	0.65375	-0.16223
1S 28.92250	0.01357	-0.00339	-0.00122	2P 13.76380	0.03936	-0.00998
2S 6.81054	0.00274	0.90297	0.29244	3P 2.92646	0.01297	0.32959
2S 15.17810	0.07693	-0.14067	-0.04564	3P 1.01565	0.00056	0.30269
3S 2.87181	0.00002	0.00350	-0.69781	3P 5.93996	0.36998	-0.11336
3S 1.67233	-0.00002	0.00057	-0.45281	3P 1.83188	-0.00273	0.52436
3S 5.86922	-0.00055	0.23387	0.15074			

POTASSIUM K(2)L(8)3S(2)3P(6)4S(2), 1S
T.E.=-0.59916174D+03 P.E.=-0.11983254D+04 K.E.= 0.59916364D+03 V.T.=-0.19999968D+01

S	1S	2S	3S	4S	P	2P	3P
BASIS/ORB E	-133.41306	-14.36594	-1.62885	-0.01018	BASIS/ORB E	-11.39927	-0.83446
1S 19.10140	-0.93428	-0.27373	0.09160	-0.01250	2P 8.65250	0.66828	-0.20593
1S 31.03670	-0.01631	-0.00210	-0.00002	0.00005	2P 15.28720	0.04077	-0.01212
2S 16.70060	-0.06155	-0.14405	0.04941	-0.00655	3P 6.91281	0.34764	-0.13477
2S 7.58500	-0.00257	0.96848	-0.34368	0.04638	3P 3.44500	0.01328	0.44812
3S 6.60786	0.00081	0.17048	-0.20565	0.03208	3P 2.26213	-0.00456	0.48310
3S 3.99350	-0.00023	0.00040	0.46742	-0.07622	3P 1.66856	0.00142	0.18819
3S 2.63830	0.00022	0.00707	0.63029	-0.09234			
4S 2.56824	-0.00009	-0.00332	0.09558	-0.00742			
4S 0.35204	0.00000	0.00004	0.00116	0.39228			
4S 1.26523	0.00000	0.00036	0.01226	0.24394			
4S 0.70452	-0.00000	-0.00015	-0.00414	0.56584			

SCANDIUM K(2)L(8)3S(2)3P(6)4S(1)3D(3), 5F
T.E.=-0.75959416D+03 P.E.=-0.15191967D+04 K.E.= 0.75960258D+03 V.T.=-0.19999889D+01

S	1S	2S	3S	4S	P	2P	3P	D	3D
BASIS/ORB E	-165.63589	-18.79775	-2.28079	-0.05069	BASIS/ORB E	-15.38901	-1.30070	BASIS/ORB E	0.01513
1S 33.23500	-0.02047	0.00113	0.00028	0.00026	2P 16.53770	0.04584	-0.01469	3D 9.91594	0.00890
1S 20.88320	-0.94488	0.28661	0.10049	-0.01974	2P 9.60190	0.68465	-0.23089	3D 5.28852	0.06800
2S 18.12350	-0.04354	0.14535	0.05705	-0.00993	3P 7.87679	0.31870	-0.14473	3D 3.08552	0.27680
2S 8.48943	-0.00389	-1.00110	-0.38349	0.07117	3P 4.22985	0.01483	0.37319	3D 1.42520	0.46525
3S 7.42737	0.00242	-0.14633	-0.22026	0.05512	3P 2.93731	-0.00424	0.55109	3D 0.51378	0.52167
3S 4.76561	-0.00155	-0.00176	0.40051	-0.10980	3P 2.00587	0.00108	0.20542		
3S 3.22922	0.00103	-0.00447	0.75353	-0.13528					
4S 2.45807	-0.00043	0.00152	0.07342	-0.03495					
4S 1.60010	0.00018	-0.00072	-0.00556	0.36934					
4S 0.89199	-0.00006	0.00021	0.00075	0.60876					
4S 0.51134	0.00002	-0.00008	-0.00084	0.15819					

See page 183 for Explanation of Tables and Notes for Tables 32, 42, and 43