

ROOTHAAN-HARTREE-FOCK ATOMIC WAVEFUNCTIONS

TABLE 2 (3). HARTREE-FOCK FUNCTIONS FOR POSITIVE IONS.

PHOSPHORUS K(2)L(8)3S(2)3P(2) -3P  
 T.E.=-0.34034959D+03 P.E.=-0.68C69365D+03 K.E.= 0.34034406D+03 V.T.=-0.20000163D+01

S		1S		2S		3S		P		2P		3P	
BASIS/ORB E													
1S	15.29030	-80.38155	0.90282	-7.91509	-1.03401	0.06967	2P	6.46199	-5.80262	-0.72003			
1S	24.54860	0.02003	-0.00585	0.93148	0.00208	2P	12.31770	0.03898	0.66290	-0.17746			
2S	5.68698	0.00496	0.93148	-0.12784	-0.29598	3P	2.02237	0.00931	0.03898	-0.00971			
2S	13.77400	0.09302	-0.12784	0.04078	0.04078	3P	1.34371	-0.00224	0.00931	0.58876			
3S	2.40272	0.00062	0.00160	0.60037	0.60037	3P	4.84290	0.37205	0.00062	-0.48308			
3S	1.62738	-0.00029	-0.00011	0.51897	0.51897								
3S	4.76941	-0.00182	0.18734	-0.12664	-0.12664								

SULFUR K(2)L(8)3S(2)3P(3) -4S  
 T.E.=-0.39717296D+03 P.E.=-0.79434200D+03 K.E.= 0.39716904D+03 V.T.=-0.20000099D+01

S		1S		2S		3S		P		2P		3P	
BASIS/ORB E													
1S	16.61110	-92.43411	0.87854	-9.42767	-1.24006	0.06764	2P	6.87921	-7.10393	-0.86169			
1S	24.51550	0.02262	-0.01175	-0.23309	0.24006	0.00501	2P	12.94140	0.68387	-0.19398			
2S	6.02289	0.00411	0.97585	0.97585	-0.32790	-0.32790	3P	2.33228	0.04332	-0.01134			
2S	15.00660	0.11829	-0.14C80	-0.14C80	0.04816	0.04816	3P	1.53607	0.00627	0.57242			
3S	2.72748	0.00037	0.00085	0.00085	0.60312	0.60312	3P	5.26386	-0.00094	0.50786			
3S	1.82072	-0.00015	0.00051	0.00051	0.53665	0.53665			0.34162	-0.10538			
3S	5.04320	-0.00137	0.13854	-0.12860	-0.12860								

CHLORINE K(2)L(8)3S(2)3P(4) - 3P  
 T.E.=-0.45904841D+03 P.E.=-0.91809217D+03 K.E.= 0.45904376D+03 V.T.=-0.20000101D+01

S		1S		2S		3S		P		2P		3P	
BASIS/ORB E													
1S	16.41090	-105.36099	0.91179	-11.07623	-1.47010	-0.08505	2P	7.49526	-8.53913	-0.93879			
1S	23.56000	0.06669	-0.01276	-0.26596	0.08505	-0.00283	2P	13.71160	0.67402	-0.19950			
2S	7.13038	0.00610	0.82157	0.82157	-0.00283	-0.00283	3P	2.64828	0.04201	-0.01120			
2S	14.87010	0.02736	-0.12810	-0.12810	0.27571	0.27571	3P	1.65706	0.00879	0.57298			
3S	2.93941	0.00050	0.00866	0.00866	-0.63782	-0.63782	3P	5.82970	-0.00104	0.52126			
3S	1.97300	-0.00025	-0.00165	-0.00165	-0.49262	-0.49262			0.34845	-0.11454			
3S	6.16710	-0.00208	0.32495	0.32495	0.19392	0.19392							

ARGON K(2)L(8)3S(2)3P(5) - 2P  
 T.E.=-0.52627435D+03 P.E.=-0.10525452D+04 K.E.= 0.52627086D+03 V.T.=-0.20000066D+01

S		1S		2S		3S		P		2P		3P	
BASIS/ORB E													
1S	18.25010	-119.13381	0.92239	-12.83628	-1.71135	0.08447	2P	7.95043	-10.08383	-1.04543			
1S	29.44590	0.01582	0.00433	0.26244	0.08447	0.00137	2P	14.19760	0.68234	-0.20940			
2S	7.26099	0.00286	-0.90535	-0.90535	-0.00137	-0.00137	3P	2.95647	0.04695	-0.01291			
2S	16.15690	0.07578	0.14294	0.14294	-0.31873	-0.31873	3P	1.79986	0.00922	0.57519			
3S	3.29566	0.00003	-0.00758	-0.00758	0.04957	0.04957	3P	6.30014	-0.00048	0.52964			
3S	2.18528	-0.00003	0.00072	0.00072	0.61185	0.61185			0.33055	-0.11664			
3S	6.40657	-0.00068	-0.22485	-0.22485	0.53681	0.53681							

POTASSIUM K(2)L(8)3S(2)3P(6) - 1S  
 T.E.=-0.59901730D+03 P.E.=-0.11980285D+04 K.E.= 0.59901120D+03 V.T.=-0.20000102D+01

S		1S		2S		3S		P		2P		3P	
BASIS/ORB E													
1S	18.98260	-133.75338	0.93931	-14.70914	-1.96444	0.08889	2P	8.61735	-11.73922	-1.17109			
1S	31.39050	0.01789	-0.00171	-0.27701	0.08889	0.00173	2P	15.19580	0.67152	-0.20999			
2S	7.30079	0.00420	1.04565	1.04565	-0.00171	-0.00171	3P	3.24817	0.04224	-0.01178			
2S	16.70010	0.05305	-0.13733	-0.13733	-0.39368	-0.39368	3P	1.94563	0.01009	0.58221			
3S	3.88331	0.00135	-0.00664	-0.00664	0.05415	0.05415	3P	6.88378	-0.00196	0.52976			
3S	2.40881	-0.00037	0.00268	0.00268	0.64114	0.64114			0.34429	-0.12638			
3S	5.70995	-0.00255	0.08655	0.08655	0.61485	0.61485							

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