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Note

Tables of Overlap Integrals

L. Klasinc, D. Schulte-Frohlinde, and M. Randić°*

Kernforschungszentrum Karlsruhe, Institut für Strahlenchemie, Karlsruhe, Deutschland and
°Institute »Ruđer Bošković«, Zagreb, Croatia, Yugoslavia

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Tables of overlap integrals for bonds between the first row atoms and their hydrides are given. They are based on atomic orbitals suggested by Clementi, which provide a more reliable guide to the description of bonds than do Slater orbitals. The region of interatomic distances is limited so as to cover known bond lengths found in the literature.

Ever since the pioneer work of Mulliken, it has been recognized that the numerical value of the overlap integral gives a good deal of information about the strength of the bond between two atoms. In this paper we present tables of overlap integrals between Clementi orbitals[1] for bonds involving boron, carbon, nitrogen, oxygen and fluorine. Clementi orbitals are considerably more accurate than Slater functions, and are still sufficiently simple so that one can anticipate their wider use in semiempirical molecular calculations, and generally in the discussion of chemical bonds. We feel, therefore, that a tabulation of bond overlap integrals based on Clementi functions may find wider use. These tables provide a more reliable guide to overlap integrals than the tables of Mulliken, Rieke, Orloff and Orloff[2], the first extensive tables of overlap integrals published some years ago, which are based on Slater orbitals, and which are still quoted. The limitations of Slater orbitals became apparent long ago, and the best would be to use truly self-consistent-field atomic orbitals. The orbitals used in these tables are not so accurate as truly self-consistent-field orbitals, but they are nearly so, and the differences would not be important. There are several reasons for refraining from the very high precision associated with the most accurate functions. The interatomic distances and bond angles are known very precisely in a few cases only. An uncertainty of $\pm$ 0.01 Å, for example, frequently changes the values of the basic atomic integrals by approximately $\pm$ 0.01, about 2—3% of their total values. Furthermore, in many molecules, the geometry is not known experimentally at all. It is also likely that very accurate functions obtained for atoms are not equally accurate when transferred to molecules. Finally, one could argue that the quality of the questions to be discussed and answered by considering overlap integrals does not demand high accuracy of the assumed functions.

Tables I—III contain representative bond overlaps for homopolar bonds, heteropolar bonds, and for hydrides respectively. The results are based on bond

* On leave from Institute »Ruđer Bošković«, Zagreb, Yugoslavia.

distances obtained from »*Tables of Interatomic Distances*«[3]. The remaining Tables contain the numerical results for a suitably selected region of interatomic distances. We have chosen an interval for the internuclear distance which covers all possible extreme cases of known bond lengths found in the literature. However, at the present time the tables do not contain information on atomic

TABLE I.: BASIC OVEPLAR INTEGRALS FOR HOMOPOLAR BONDS

Bond	R(Å)	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
B - B	1.590	0.4768	0.4968	0.2012	0.3895
C ≡ C	1.205	0.5126	0.4964	0.1796	0.4044
C = C	1.335	0.4493	0.4707	0.2311	0.3449
C = C	1.395	0.4211	0.4560	0.2482	0.3197
C - C	1.540	0.3567	0.4154	0.2750	0.2648
N ≡ N	1.130	0.4437	0.4585	0.2385	0.3278
N = N	1.250	0.3788	0.4205	0.2679	0.2719
N - N	1.460	0.2794	0.3450	0.2799	0.1929
O = O	1.275	0.2683	0.3454	0.2684	0.1975
O - O	1.480	0.1832	0.2634	0.2501	0.1339
F - F	1.418	0.1397	0.2184	0.2260	0.1055

TABLE II.: BASIC OVERLAP INTEGRALS FOR HETEROPOLAR BONDS

Bond	R(Å)	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
B - C	1.560	0.4142	0.4990	0.4048	0.2378	0.3182
B ≡ N	1.280	0.4667	0.5450	0.3635	0.1761	0.3511
B - N	1.415	0.4090	0.5105	0.3475	0.2173	0.2987
C ≡ N	1.160	0.4780	0.4316	0.5161	0.2050	0.3626
C = N	1.340	0.3877	0.3916	0.4627	0.2576	0.2824
C - N	1.470	0.3285	0.3551	0.4177	0.2738	0.2338
C = O	1.230	0.3858	0.3660	0.4784	0.2365	0.2862
C - O	1.430	0.2934	0.3145	0.4013	0.2609	0.2110
C - F	1.380	0.2703	0.2783	0.3874	0.2460	0.1915
N = O	1.220	0.3429	0.3790	0.4179	0.2659	0.2493
N - O	1.360	0.2748	0.3299	0.3595	0.2721	0.1958
N - F	1.360	0.2336	0.2801	0.3317	0.2588	0.1652

TABLE III.: BASIC OVERLAP INTEGRALS FOR HYDRIDE BONDS

Bond	R(Å)	$(2s,1s_H)$	$(2p,1s_H)$
B - H	1.210	0.5712	0.5536
C - H	1.080	0.5767	0.5065
N - H	1.020	0.5484	0.4492
O - H	0.960	0.5207	0.4105
F - H	0.918	0.4884	0.3696

overlap integrals for distances which are found when considering interactions of non-bonded atoms.

The tables IV—XVIII contain overlap integrals for bonds between the first row atoms, and tables XIX—XXIII contain overlap integrals for hydrides of the first row atoms. The first column gives the internuclear distance in angstroms, the remaining columns give the basic overlap integrals between orbitals ψ_{2s} and ψ_{2p}: (2s, 2s), (2s, 2p), (2p, 2s), $(2p,2p)_\sigma$ and $(2p,2p)_\pi$

TABLE IV. : BASIC OVERLAP INTEGRALS FOR BORON-BORON BONDS

R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.65	0.45339	0.48651	0.22067	0.36762	1.77	0.40795	0.46268	0.25158	0.32663
					1.78	0.40426	0.46052	0.25371	0.32338
1.66	0.44953	0.48468	0.22364	0.36407	1.79	0.40059	0.45835	0.25576	0.32015
1.67	0.44568	0.48282	0.22654	0.36054	1.80	0.39694	0.45615	0.25776	0.31694
1.68	0.44184	0.48093	0.22937	0.35704					
1.69	0.43801	0.47901	0.23212	0.35356	1.81	0.39330	0.45393	0.25968	0.31376
1.70	0.43420	0.47706	0.23480	0.35011	1.82	0.38968	0.45170	0.26155	0.31060
					1.83	0.38608	0.44944	0.26335	0.30747
1.71	0.43041	0.47509	0.23741	0.34668	1.84	0.38250	0.44717	0.26509	0.30437
1.72	0.42662	0.47308	0.23994	0.34327	1.85	0.37894	0.44488	0.26677	0.30128
1.73	0.42286	0.47105	0.24241	0.33990					
1.74	0.41911	0.46899	0.24481	0.33654	1.86	0.37539	0.44257	0.26838	0.29823
1.75	0.41537	0.46691	0.24713	0.33321	1.87	0.37187	0.44024	0.26994	0.29519
					1.88	0.36836	0.43790	0.27144	0.29218
1.76	0.41165	0.46481	0.24939	0.32991	1.89	0.36487	0.43554	0.27288	0.28920

TABLE V. : BASIC OVERLAP INTEGRALS FOR BORON-CARBON BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.50	0.43882	0.41537	0.51378	0.22210	0.34011	1.57	0.41017	0.40290	0.49638	0.24007	0.31463
						1.58	0.40614	0.40099	0.49378	0.24231	0.31111
1.51	0.43468	0.41369	0.51139	0.22492	0.33638	1.59	0.40214	0.39904	0.49115	0.24447	0.30762
1.52	0.43055	0.41198	0.50897	0.22765	0.33268	1.60	0.39815	0.39707	0.48850	0.24655	0.30417
1.53	0.42644	0.41023	0.50651	0.23030	0.32901						
1.54	0.42235	0.40845	0.50402	0.23287	0.32537	1.61	0.39418	0.39507	0.48582	0.24855	0.30074
1.55	0.41827	0.40663	0.50150	0.23535	0.32176	1.62	0.39024	0.39305	0.48312	0.25048	0.29734
						1.63	0.38631	0.39100	0.48040	0.25234	0.29398
1.56	0.41421	0.40478	0.49896	0.23775	0.31818	1.64	0.38240	0.38892	0.47766	0.25411	0.29064

TABLE VI. : BASIC OVERLAP INTEGRALS FOR BORON-NITROGEN BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.25	0.47976	0.36570	0.55152	0.16444	0.36362	1.37	0.42797	0.35376	0.52283	0.20553	0.31546
						1.38	0.42373	0.35244	0.52016	0.20830	0.31168
1.26	0.47540	0.36501	0.54940	0.16845	0.35942	1.39	0.41950	0.35107	0.51745	0.21097	0.30793
1.27	0.47104	0.36426	0.54723	0.17235	0.35525	1.40	0.41529	0.34967	0.51470	0.21355	0.30421
1.28	0.46669	0.36345	0.54501	0.17614	0.35111						
1.29	0.46235	0.36258	0.54273	0.17982	0.34701	1.41	0.41109	0.34822	0.51192	0.21604	0.30053
1.30	0.45801	0.36166	0.54040	0.18339	0.34294	1.42	0.40691	0.34674	0.50911	0.21843	0.29688
						1.43	0.40275	0.34521	0.50627	0.22074	0.29327
1.31	0.45369	0.36068	0.53803	0.18686	0.33891	1.44	0.39861	0.34365	0.50339	0.22295	0.28969
1.32	0.44937	0.35965	0.53560	0.19023	0.33491	1.45	0.39448	0.34205	0.50049	0.22508	0.28615
1.33	0.44507	0.35857	0.53313	0.19349	0.33095						
1.34	0.44077	0.35744	0.53062	0.19665	0.32703	1.46	0.39038	0.34041	0.49757	0.22713	0.28264
1.35	0.43649	0.35626	0.52807	0.19971	0.32314	1.47	0.38629	0.33874	0.49461	0.22909	0.27917
						1.48	0.38222	0.33704	0.49163	0.23097	0.27573
1.36	0.43222	0.35503	0.52547	0.20267	0.31928	1.49	0.37818	0.33530	0.48863	0.23276	0.27232

TABLE VII. : BASIC OVERLAP INTEGRALS FOR BORON-OXYGEN BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.15	0.46107	0.32127	0.54800	0.13734	0.35309	1.27	0.41009	0.31488	0.51740	0.18070	0.30457
						1.28	0.40589	0.31398	0.51454	0.18362	0.30077
1.16	0.45680	0.32109	0.54574	0.14157	0.34884	1.29	0.40171	0.31302	0.51165	0.18644	0.29701
1.17	0.45253	0.32084	0.54343	0.14569	0.34463	1.30	0.39754	0.31201	0.50872	0.18916	0.29328
1.18	0.44826	0.32052	0.54106	0.14969	0.34046						
1.19	0.44400	0.32013	0.53863	0.15358	0.33632	1.31	0.39338	0.31096	0.50576	0.19178	0.28958
1.20	0.43973	0.31968	0.53615	0.15735	0.33223	1.32	0.38924	0.30986	0.50277	0.19431	0.28593
						1.33	0.38511	0.30871	0.49974	0.19674	0.28231
1.21	0.43548	0.31917	0.53361	0.16101	0.32817	1.34	0.38100	0.30752	0.49668	0.19908	0.27872
1.22	0.43123	0.31860	0.53103	0.16456	0.32414	1.35	0.37691	0.30629	0.49359	0.20133	0.27518
1.23	0.42698	0.31797	0.52839	0.16800	0.32015						
1.24	0.42274	0.31728	0.52571	0.17133	0.31620	1.36	0.37283	0.30501	0.49048	0.20349	0.27166
1.25	0.41852	0.31654	0.52298	0.17456	0.31229	1.37	0.36878	0.30369	0.48734	0.20556	0.26819
						1.38	0.36474	0.30234	0.48418	0.20754	0.26475
1.26	0.41430	0.31574	0.52021	0.17768	0.30841	1.39	0.36072	0.30095	0.48099	0.20944	0.26134

TABLE VIII. : BASIC OVERLAP INTEGRALS FOR BORON-FLUORINE BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.25	0.36618	0.26979	0.48664	0.17770	0.26372
1.26	0.36218	0.26892	0.48350	0.18000	0.26021
1.27	0.35819	0.26801	0.48032	0.18220	0.25674
1.28	0.35422	0.26706	0.47712	0.18432	0.25330
1.29	0.35026	0.26605	0.47389	0.18634	0.24990
1.30	0.34632	0.26501	0.47064	0.18827	0.24654
1.31	0.34240	0.26392	0.46736	0.19012	0.24321
1.32	0.33850	0.26279	0.46406	0.19187	0.23992
1.33	0.33461	0.26163	0.46075	0.19355	0.23667
1.34	0.33075	0.26042	0.45742	0.19514	0.23345
1.35	0.32690	0.25918	0.45407	0.19665	0.23027
1.36	0.32308	0.25790	0.45070	0.19808	0.22713
1.37	0.31928	0.25658	0.44732	0.19944	0.22402
1.38	0.31549	0.25524	0.44393	0.20071	0.22094
1.39	0.31174	0.25386	0.44053	0.20191	0.21791
1.40	0.30800	0.25245	0.43711	0.20304	0.21490
1.41	0.30429	0.25102	0.43369	0.20410	0.21194
1.42	0.30060	0.24955	0.43026	0.20508	0.20900
1.43	0.29694	0.24806	0.42682	0.20600	0.20610
1.44	0.29330	0.24654	0.42338	0.20685	0.20324
1.45	0.28969	0.24500	0.41993	0.20763	0.20041
1.46	0.28610	0.24343	0.41648	0.20835	0.19761
1.47	0.28254	0.24184	0.41303	0.20900	0.19485
1.48	0.27901	0.24023	0.40957	0.20959	0.19212
1.49	0.27550	0.23859	0.40612	0.21012	0.18942

TABLE IX. : BASIC OVERLAP INTEGRALS FOR CARBON-CARBON BONDS

R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.15	0.54001	0.50400	0.15127	0.43166
1.16	0.53502	0.50279	0.15672	0.42661
1.17	0.53003	0.50150	0.16204	0.42160
1.18	0.52505	0.50014	0.16723	0.41663
1.19	0.52008	0.49870	0.17227	0.41171
1.20	0.51511	0.49719	0.17718	0.40682
1.21	0.51016	0.49561	0.18196	0.40197
1.22	0.50521	0.49397	0.18661	0.39717
1.23	0.50027	0.49225	0.19112	0.39240
1.24	0.49535	0.49047	0.19551	0.38768
1.25	0.49044	0.48863	0.19977	0.38300
1.26	0.48554	0.48673	0.20391	0.37836
1.27	0.48066	0.48477	0.20792	0.37376
1.28	0.47579	0.48275	0.21181	0.36920
1.29	0.47094	0.48067	0.21557	0.36468
1.30	0.46610	0.47855	0.21922	0.36020
1.31	0.46128	0.47636	0.22275	0.35576
1.32	0.45648	0.47413	0.22616	0.35137
1.33	0.45170	0.47185	0.22946	0.34701
1.34	0.44694	0.46953	0.23264	0.34270
1.35	0.44220	0.46715	0.23572	0.33843
1.36	0.43748	0.46474	0.23868	0.33419
1.37	0.43278	0.46228	0.24153	0.33000
1.38	0.42810	0.45978	0.24428	0.32585
1.39	0.42345	0.45724	0.24692	0.32174
1.40	0.41882	0.45466	0.24946	0.31767
1.41	0.41421	0.45205	0.25189	0.31364
1.42	0.40963	0.44940	0.25423	0.30965
1.43	0.40507	0.44672	0.25646	0.30569
1.44	0.40054	0.44401	0.25860	0.30178
1.45	0.39604	0.44127	0.26064	0.29791
1.46	0.39156	0.43850	0.26259	0.29408
1.47	0.38711	0.43570	0.26444	0.29029
1.48	0.38268	0.43287	0.26621	0.28653
1.49	0.37829	0.43002	0.26788	0.28282
1.50	0.37392	0.42715	0.26946	0.27914
1.51	0.36958	0.42425	0.27096	0.27550
1.52	0.36527	0.42133	0.27237	0.27190
1.53	0.36099	0.41840	0.27370	0.26834
1.54	0.35674	0.41544	0.27495	0.26482
1.55	0.35252	0.41247	0.27611	0.26133
1.56	0.34833	0.40948	0.27720	0.25788
1.57	0.34417	0.40647	0.27821	0.25447
1.58	0.34004	0.40345	0.27914	0.25110
1.59	0.33594	0.40042	0.27999	0.24776

TABLE X. : BASIC OVERLAP INTEGRALS FOR CARBON-NITROGEN BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.10	0.50948	0.44050	0.52975	0.17772	0.39287
1.11	0.50420	0.43920	0.52765	0.18265	0.38771
1.12	0.49893	0.43783	0.52548	0.18742	0.38260
1.13	0.49367	0.43637	0.52323	0.19203	0.37753
1.14	0.48842	0.43484	0.52090	0.19650	0.37252
1.15	0.48319	0.43324	0.51851	0.20083	0.36755
1.16	0.47797	0.43156	0.51605	0.20500	0.36263
1.17	0.47277	0.42982	0.51352	0.20904	0.35776
1.18	0.46758	0.42801	0.51093	0.21293	0.35294
1.19	0.46241	0.42613	0.50828	0.21669	0.34817
1.20	0.45727	0.42419	0.50557	0.22030	0.34345
1.21	0.45214	0.42219	0.50280	0.22379	0.33877
1.22	0.44703	0.42013	0.49998	0.22714	0.33415
1.23	0.44195	0.41802	0.49711	0.23036	0.32957
1.24	0.43689	0.41585	0.49419	0.23345	0.32505
1.25	0.43185	0.41362	0.49122	0.23641	0.32057
1.26	0.42684	0.41135	0.48821	0.23925	0.31613
1.27	0.42185	0.40903	0.48515	0.24197	0.31175
1.28	0.41689	0.40666	0.48205	0.24457	0.30741
1.29	0.41195	0.40425	0.47892	0.24705	0.30312
1.30	0.40704	0.40179	0.47574	0.24941	0.29888
1.31	0.40217	0.39929	0.47253	0.25166	0.29469
1.32	0.39732	0.39676	0.46929	0.25380	0.29054
1.33	0.39250	0.39418	0.46601	0.25583	0.28644
1.34	0.38771	0.39157	0.46270	0.25775	0.28239
1.35	0.38295	0.38893	0.45937	0.25956	0.27838
1.36	0.37822	0.38625	0.45601	0.26127	0.27442
1.37	0.37353	0.38354	0.45262	0.26288	0.27050
1.38	0.36887	0.38081	0.44921	0.26439	0.26663
1.39	0.36424	0.37804	0.44578	0.26580	0.26281
1.40	0.35965	0.37525	0.44233	0.26711	0.25903
1.41	0.35508	0.37244	0.43886	0.26833	0.25529

Continued on next page.

TABLE X. : BASIC OVERLAP INTEGRALS FOR CARBON-NITROGEN BONDS (CONTINUED)

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.42	0.35056	0.36960	0.43538	0.26946	0.25160	1.51	0.31144	0.34325	0.40346	0.27576	0.22032
1.43	0.34607	0.36674	0.43187	0.27050	0.24795	1.52	0.30727	0.34026	0.39987	0.27606	0.21706
1.44	0.34161	0.36386	0.42836	0.27144	0.24435	1.53	0.30315	0.33725	0.39629	0.27629	0.21383
1.45	0.33719	0.36096	0.42483	0.27231	0.24079	1.54	0.29906	0.33425	0.39270	0.27646	0.21065
						1.55	0.29501	0.33123	0.38911	0.27655	0.20751
1.46	0.33281	0.35804	0.42129	0.27308	0.23727						
1.47	0.32846	0.35511	0.41774	0.27378	0.23380	1.56	0.29100	0.32821	0.38552	0.27658	0.20440
1.48	0.32415	0.35217	0.41418	0.27439	0.23036	1.57	0.28703	0.32518	0.38194	0.27654	0.20134
1.49	0.31987	0.34921	0.41061	0.27492	0.22697	1.58	0.28310	0.32215	0.37835	0.27643	0.19832
1.50	0.31564	0.34623	0.40703	0.27538	0.22363	1.59	0.27920	0.31912	0.37477	0.27627	0.19533

TABLE XI. : BASIC OVERLAP INTEGRALS FOR CARBON-OXYGEN BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.10	0.45289	0.39044	0.52271	0.19625	0.34586	1.30	0.35184	0.34935	0.45219	0.24951	0.25771
1.11	0.44760	0.38895	0.51962	0.20018	0.34095	1.31	0.34712	0.34682	0.44834	0.25094	0.25383
1.12	0.44232	0.38738	0.51647	0.20396	0.33611	1.32	0.34244	0.34426	0.44448	0.25227	0.25001
1.13	0.43706	0.38574	0.51326	0.20759	0.33131	1.33	0.33779	0.34167	0.44060	0.25350	0.24622
1.14	0.43183	0.38404	0.51000	0.21108	0.32657	1.34	0.33319	0.33906	0.43671	0.25464	0.24249
1.15	0.42662	0.38227	0.50668	0.21443	0.32188	1.35	0.32862	0.33642	0.43281	0.25568	0.23880
1.16	0.42143	0.38044	0.50331	0.21764	0.31724	1.36	0.32409	0.33375	0.42890	0.25663	0.23517
1.17	0.41626	0.37854	0.49989	0.22072	0.31266	1.37	0.31960	0.33106	0.42498	0.25748	0.23157
1.18	0.41113	0.37659	0.49643	0.22367	0.30812	1.38	0.31515	0.32835	0.42106	0.25825	0.22803
1.19	0.40602	0.37458	0.49292	0.22648	0.30364	1.39	0.31073	0.32562	0.41713	0.25894	0.22452
1.20	0.40093	0.37252	0.48938	0.22917	0.29921	1.40	0.30636	0.32288	0.41320	0.25954	0.22107
1.21	0.39588	0.37040	0.48580	0.23173	0.29484	1.41	0.30203	0.32011	0.40926	0.26005	0.21766
1.22	0.39086	0.36824	0.48218	0.23417	0.29051	1.42	0.29775	0.31733	0.40533	0.26049	0.21429
1.23	0.38586	0.36602	0.47852	0.23649	0.28623	1.43	0.29350	0.31454	0.40139	0.26085	0.21097
1.24	0.38090	0.36376	0.47484	0.23869	0.28201	1.44	0.28929	0.31173	0.39746	0.26113	0.20769
1.25	0.37597	0.36146	0.47113	0.24077	0.27784	1.45	0.28513	0.30891	0.39353	0.26134	0.20446
1.26	0.37108	0.35911	0.46739	0.24274	0.27371	1.46	0.28100	0.30608	0.38961	0.26147	0.20127
1.27	0.36622	0.35673	0.46362	0.24459	0.26964	1.47	0.27692	0.30325	0.38569	0.26153	0.19812
1.28	0.36139	0.35430	0.45983	0.24634	0.26561	1.48	0.27288	0.30040	0.38178	0.26153	0.19502
1.29	0.35660	0.35184	0.45602	0.24798	0.26164	1.49	0.26889	0.29755	0.37787	0.26146	0.19195

TABLE XII.: BASIC OVERLAP INTEGRALS FOR CARBON-FLUORINE BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.25	0.32767	0.31075	0.44142	0.23797	0.23666	1.35	0.28288	0.28607	0.39986	0.24544	0.20117
1.26	0.32301	0.30841	0.43729	0.23914	0.23288	1.36	0.27863	0.28349	0.39570	0.24571	0.19788
1.27	0.31839	0.30603	0.43314	0.24021	0.22916	1.37	0.27443	0.28088	0.39155	0.24590	0.19464
1.28	0.31380	0.30362	0.42899	0.24118	0.22549	1.38	0.27027	0.27827	0.38741	0.24602	0.19145
1.29	0.30926	0.30119	0.42483	0.24205	0.22187	1.39	0.26615	0.27564	0.38328	0.24607	0.18830
1.30	0.30476	0.29873	0.42067	0.24284	0.21830	1.40	0.26208	0.27300	0.37916	0.24604	0.18520
1.31	0.30030	0.29624	0.41651	0.24353	0.21478	1.41	0.25805	0.27035	0.37505	0.24595	0.18214
1.32	0.29588	0.29373	0.41234	0.24413	0.21130	1.42	0.25407	0.26769	0.37095	0.24578	0.17913
1.33	0.29150	0.29120	0.40818	0.24465	0.20788	1.43	0.25013	0.26502	0.36686	0.24555	0.17616
1.34	0.28717	0.28864	0.40402	0.24508	0.20450	1.44	0.24623	0.26235	0.36279	0.24526	0.17323

TABLE XIII. : BASIC OVERLAP INTEGRALS FOR NITROGEN-NITROGEN BONDS

R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.05	0.48942	0.47925	0.20698	0.36980	1.12	0.44932	0.46132	0.23515	0.33283
					1.13	0.44369	0.45849	0.23853	0.32779
1.06	0.48362	0.47691	0.21151	0.36434	1.14	0.43810	0.45559	0.24175	0.32281
1.07	0.47784	0.47450	0.21587	0.35894	1.15	0.43253	0.45264	0.24483	0.31788
1.08	0.47209	0.47201	0.22005	0.35359					
1.09	0.46636	0.46944	0.22407	0.34831	1.16	0.42700	0.44963	0.24775	0.31302
1.10	0.46065	0.46680	0.22793	0.34309	1.17	0.42149	0.44657	0.25053	0.30822
					1.18	0.41603	0.44345	0.25317	0.30347
1.11	0.45497	0.46410	0.23162	0.33793	1.19	0.41059	0.44030	0.25567	0.29878

Continued on next page.

TABLE XIII.': BASIC OVERLAP INTEGRALS FOR NITROGEN-NITROGEN BONDS (CONTINUED)

R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.20	0.40520	0.43709	0.25803	0.29415	1.50	0.26276	0.33036	0.27798	0.18028
1.21	0.39983	0.43385	0.26025	0.28958	1.51	0.25872	0.32672	0.27734	0.17724
1.22	0.39451	0.43056	0.26235	0.28506	1.52	0.25473	0.32310	0.27664	0.17425
1.23	0.38922	0.42724	0.26431	0.28060	1.53	0.25079	0.31948	0.27588	0.17131
1.24	0.38397	0.42388	0.26615	0.27620	1.54	0.24689	0.31588	0.27506	0.16841
1.25	0.37877	0.42048	0.26787	0.27186	1.55	0.24303	0.31229	0.27419	0.16555
1.26	0.37360	0.41706	0.26947	0.26757	1.56	0.23923	0.30871	0.27326	0.16273
1.27	0.36847	0.41361	0.27095	0.26333	1.57	0.23547	0.30514	0.27228	0.15996
1.28	0.36338	0.41013	0.27231	0.25915	1.58	0.23176	0.30159	0.27125	0.15723
1.29	0.35834	0.40662	0.27356	0.25503	1.59	0.22809	0.29806	0.27018	0.15454
1.30	0.35333	0.40309	0.27470	0.25096	1.60	0.22447	0.29454	0.26905	0.15189
1.31	0.34838	0.39955	0.27573	0.24694	1.61	0.22090	0.29104	0.26788	0.14927
1.32	0.34346	0.39598	0.27665	0.24298	1.62	0.21737	0.28755	0.26667	0.14670
1.33	0.33859	0.39239	0.27748	0.23907	1.63	0.21389	0.28408	0.26541	0.14417
1.34	0.33376	0.38879	0.27820	0.23521	1.64	0.21045	0.28064	0.26411	0.14168
1.35	0.32898	0.38518	0.27882	0.23140	1.65	0.20706	0.27721	0.26278	0.13922
1.36	0.32424	0.38155	0.27935	0.22765	1.66	0.20371	0.27380	0.26140	0.13680
1.37	0.31955	0.37792	0.27979	0.22395	1.67	0.20040	0.27041	0.25999	0.13442
1.38	0.31490	0.37427	0.28013	0.22030	1.68	0.19714	0.26704	0.25855	0.13208
1.39	0.31030	0.37062	0.28039	0.21669	1.69	0.19393	0.26370	0.25707	0.12977
1.40	0.30574	0.36696	0.28055	0.21314	1.70	0.19076	0.26037	0.25556	0.12750
1.41	0.30123	0.36330	0.28064	0.20964	1.71	0.18763	0.25707	0.25402	0.12527
1.42	0.29677	0.35963	0.28064	0.20619	1.72	0.18454	0.25380	0.25245	0.12307
1.43	0.29236	0.35596	0.28057	0.20279	1.73	0.18150	0.25054	0.25086	0.12090
1.44	0.28799	0.35230	0.28041	0.19943	1.74	0.17850	0.24731	0.24923	0.11877
1.45	0.28367	0.34863	0.28018	0.19612	1.75	0.17554	0.24410	0.24759	0.11667
1.46	0.27939	0.34497	0.27988	0.19286	1.76	0.17262	0.24092	0.24591	0.11461
1.47	0.27516	0.34131	0.27951	0.18964	1.77	0.16974	0.23776	0.24422	0.11257
1.48	0.27098	0.33765	0.27906	0.18648	1.78	0.16691	0.23463	0.24250	0.11057
1.49	0.26685	0.33400	0.27855	0.18335	1.79	0.16411	0.23152	0.24076	0.10861

TABLE XIV.': BASIC OVERLAP INTEGRALS FOR NITROGEN-OXYGEN BOND

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.05	0.43841	0.43062	0.48364	0.22659	0.33010	1.27	0.31745	0.36182	0.39725	0.27037	0.22893
						1.28	0.31250	0.35832	0.39307	0.27094	0.22502
1.06	0.43248	0.42803	0.48015	0.23011	0.32483	1.29	0.30760	0.35480	0.38889	0.27141	0.22118
1.07	0.42657	0.42537	0.47659	0.23346	0.31963	1.30	0.30276	0.35128	0.38470	0.27178	0.21739
1.08	0.42071	0.42264	0.47298	0.23665	0.31449						
1.09	0.41488	0.41983	0.46931	0.23968	0.30942	1.31	0.29797	0.34774	0.38052	0.27205	0.21365
1.10	0.40909	0.41699	0.46559	0.24255	0.30442	1.32	0.29323	0.34419	0.37634	0.27224	0.20997
						1.33	0.28855	0.34064	0.37215	0.27233	0.20634
1.11	0.40334	0.41408	0.46182	0.24527	0.29948	1.34	0.28392	0.33708	0.36798	0.27234	0.20277
1.12	0.39762	0.41112	0.45801	0.24784	0.29460	1.35	0.27934	0.33351	0.36381	0.27226	0.19925
1.13	0.39196	0.40810	0.45415	0.25026	0.28979						
1.14	0.38633	0.40503	0.45026	0.25254	0.28504	1.36	0.27482	0.32994	0.35964	0.27210	0.19579
1.15	0.38075	0.40192	0.44633	0.25467	0.28036	1.37	0.27035	0.32637	0.35549	0.27186	0.19237
						1.38	0.26593	0.32281	0.35134	0.27154	0.18901
1.16	0.37521	0.39876	0.44236	0.25667	0.27574	1.39	0.26157	0.31924	0.34721	0.27114	0.18570
1.17	0.36972	0.39556	0.43837	0.25853	0.27118	1.40	0.25726	0.31568	0.34309	0.27068	0.18244
1.18	0.36427	0.39232	0.43434	0.26026	0.26668						
1.19	0.35887	0.38905	0.43029	0.26186	0.26225	1.41	0.25301	0.31212	0.33899	0.27014	0.17922
1.20	0.35352	0.38574	0.42622	0.26333	0.25787	1.42	0.24881	0.30856	0.33490	0.26953	0.17606
						1.43	0.24466	0.30501	0.33082	0.26886	0.17295
1.21	0.34822	0.38240	0.42213	0.26468	0.25356	1.44	0.24056	0.30147	0.32676	0.26812	0.16988
1.22	0.34296	0.37903	0.41801	0.26591	0.24931	1.45	0.23652	0.29794	0.32273	0.26732	0.16686
1.23	0.33776	0.37563	0.41389	0.26703	0.24511						
1.24	0.33260	0.37221	0.40974	0.26802	0.24098	1.46	0.23254	0.29442	0.31871	0.26646	0.16389
1.25	0.32750	0.36877	0.40559	0.26891	0.23690	1.47	0.22860	0.29092	0.31471	0.26554	0.16097
						1.48	0.22472	0.28742	0.31073	0.26456	0.15809
1.26	0.32245	0.36530	0.40142	0.26969	0.23289	1.49	0.22089	0.28394	0.30677	0.26353	0.15526

TABLE XV. : BASIC OVERLAP INTEGRALS FOR NITROGEN-FLUORINE BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.30	0.25974	0.30075	0.35836	0.26230	0.18488	1.37	0.22941	0.27671	0.32738	0.25802	0.16212
						1.38	0.22531	0.27330	0.32304	0.25713	0.15908
1.31	0.25523	0.29731	0.35387	0.26191	0.18147	1.39	0.22127	0.26990	0.31873	0.25618	0.15609
1.32	0.25078	0.29387	0.34941	0.26145	0.17811	1.40	0.21728	0.26650	0.31445	0.25517	0.15315
1.33	0.24639	0.29043	0.34496	0.26090	0.17481						
1.34	0.24206	0.28700	0.34053	0.26029	0.17156	1.41	0.21336	0.26312	0.31019	0.25411	0.15026
1.35	0.23778	0.28356	0.33612	0.25960	0.16836	1.42	0.20949	0.25975	0.30597	0.25298	0.14741
						1.43	0.20567	0.25640	0.30177	0.25181	0.14462
1.36	0.23357	0.28013	0.33174	0.25884	0.16522	1.44	0.20192	0.25306	0.29760	0.25058	0.14187

TABLE XVI. : BASIC OVERLAP INTEGRALS FOR OXYGEN-OXYGEN BONDS

R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.10	0.36183	0.41759	0.25501	0.27102	1.35	0.23420	0.31458	0.26487	0.17169
1.11	0.35599	0.41362	0.25679	0.26627	1.36	0.22991	0.31051	0.26408	0.16848
1.12	0.35021	0.40962	0.25843	0.26159	1.37	0.22569	0.30647	0.26323	0.16533
1.13	0.34448	0.40559	0.25994	0.25698	1.38	0.22153	0.30244	0.26231	0.16223
1.14	0.33881	0.40154	0.26131	0.25244	1.39	0.21743	0.29843	0.26133	0.15918
1.15	0.33321	0.39746	0.26255	0.24797	1.40	0.21339	0.29445	0.26029	0.15618
1.16	0.32766	0.39336	0.26366	0.24356	1.41	0.20941	0.29049	0.25920	0.15323
1.17	0.32218	0.38924	0.26465	0.23922	1.42	0.20549	0.28655	0.25805	0.15033
1.18	0.31675	0.38511	0.26552	0.23495	1.43	0.20164	0.28264	0.25684	0.14748
1.19	0.31139	0.38097	0.26627	0.23074	1.44	0.19784	0.27875	0.25558	0.14467
1.20	0.30609	0.37681	0.26691	0.22660	1.45	0.19410	0.27489	0.25428	0.14192
1.21	0.30085	0.37265	0.26744	0.22252	1.46	0.19042	0.27105	0.25293	0.13921
1.22	0.29568	0.36848	0.26786	0.21850	1.47	0.18680	0.26725	0.25153	0.13654
1.23	0.29057	0.36430	0.26818	0.21454	1.48	0.18324	0.26347	0.25009	0.13393
1.24	0.28552	0.36013	0.26839	0.21065	1.49	0.17973	0.25972	0.24860	0.13135
1.25	0.28054	0.35595	0.26851	0.20682	1.50	0.17628	0.25600	0.24708	0.12883
1.26	0.27562	0.35178	0.26853	0.20304	1.51	0.17289	0.25231	0.24552	0.12634
1.27	0.27076	0.34761	0.26846	0.19933	1.52	0.16956	0.24865	0.24393	0.12390
1.28	0.26597	0.34344	0.26829	0.19568	1.53	0.16627	0.24503	0.24230	0.12150
1.29	0.26124	0.33929	0.26805	0.19208	1.54	0.16305	0.24143	0.24063	0.11915
1.30	0.25658	0.33514	0.26771	0.18854	1.55	0.15988	0.23787	0.23894	0.11683
1.31	0.25197	0.33100	0.26730	0.18506	1.56	0.15676	0.23434	0.23721	0.11455
1.32	0.24744	0.32687	0.26680	0.18164	1.57	0.15369	0.23084	0.23546	0.11232
1.33	0.24296	0.32276	0.26623	0.17827	1.58	0.15068	0.22738	0.23369	0.11012
1.34	0.23855	0.31866	0.26559	0.17495	1.59	0.14771	0.22395	0.23188	0.10797

TABLE XVII. : BASIC OVERLAP INTEGRALS FOR OXYGEN-FLUORINE BONDS

R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	(2p,2s)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.35	0.19673	0.26679	0.28994	0.25179	0.14510	1.42	0.17039	0.24021	0.26087	0.24155	0.12578
						1.43	0.16688	0.23654	0.25687	0.23991	0.12321
1.36	0.19277	0.26291	0.28568	0.25047	0.14219	1.44	0.16343	0.23289	0.25289	0.23823	0.12070
1.37	0.18888	0.25905	0.28146	0.24910	0.13932	1.45	0.16005	0.22928	0.24896	0.23651	0.11823
1.38	0.18505	0.25523	0.27727	0.24768	0.13652						
1.39	0.18129	0.25143	0.27312	0.24622	0.13376	1.46	0.15672	0.22570	0.24507	0.23477	0.11581
1.40	0.17759	0.24766	0.26900	0.24470	0.13105	1.47	0.15346	0.22216	0.24121	0.23299	0.11343
						1.48	0.15025	0.21865	0.23740	0.23117	0.11109
1.41	0.17396	0.24392	0.26492	0.24315	0.12839	1.49	0.14710	0.21517	0.23362	0.22933	0.10880

TABLE XVIII. : BASIC OVERLAP INTEGRALS FOR FLUORINE-FLUORINE BONDS

R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$	R	(2s,2s)	(2s,2p)	$(2p,2p)_\sigma$	$(2p,2p)_\pi$
1.35	0.16299	0.24502	0.23875	0.12257	1.40	0.14557	0.22523	0.22949	0.10983
1.36	0.15937	0.24098	0.23697	0.11992	1.41	0.14229	0.22140	0.22753	0.10743
1.37	0.15582	0.23698	0.23516	0.11732	1.42	0.13907	0.21762	0.22555	0.10508
1.38	0.15234	0.23302	0.23330	0.11477	1.43	0.13591	0.21387	0.22354	0.10277
1.39	0.14892	0.22911	0.23141	0.11228	1.44	0.13282	0.21017	0.22150	0.10051

TABLE XIX. : BASIC OVERLAP INTEGRALS FOR HYDROGEN-BORON BONDS

R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)
1.170	0.588849	0.557946	1.236	0.559777	0.550283	1.302	0.530872	0.540361
1.172	0.587968	0.557753	1.238	0.558898	0.550008	1.304	0.530001	0.540029
1.174	0.587086	0.557555	1.240	0.558019	0.549742	1.306	0.529130	0.539692
1.176	0.586205	0.557351	1.242	0.557140	0.549466	1.308	0.528259	0.539359
1.178	0.585323	0.557148	1.244	0.556261	0.549194	1.310	0.527389	0.539018
1.180	0.584442	0.556943	1.246	0.555382	0.548913	1.312	0.526519	0.538682
1.182	0.583560	0.556738	1.248	0.554504	0.548637	1.314	0.525650	0.538341
1.184	0.582679	0.556525	1.250	0.553625	0.548353	1.316	0.524780	0.537998
1.186	0.581797	0.556316	1.252	0.552747	0.548075	1.318	0.523911	0.537653
1.188	0.580916	0.556098	1.254	0.551869	0.547784	1.320	0.523043	0.537310
1.190	0.580034	0.555887	1.256	0.550991	0.547502	1.322	0.522175	0.536959
1.192	0.579153	0.555665	1.258	0.550114	0.547210	1.324	0.521307	0.536609
1.194	0.578271	0.555438	1.260	0.549237	0.546916	1.326	0.520440	0.536255
1.196	0.577390	0.555220	1.262	0.548360	0.546625	1.328	0.519573	0.535908
1.198	0.576508	0.554991	1.264	0.547483	0.546327	1.330	0.518706	0.535551
1.200	0.575627	0.554766	1.266	0.546606	0.546033	1.332	0.517840	0.535192
1.202	0.574746	0.554532	1.268	0.545730	0.545731	1.334	0.516974	0.534836
1.204	0.573865	0.554302	1.270	0.544853	0.545432	1.336	0.516109	0.534474
1.206	0.572983	0.554064	1.272	0.543978	0.545127	1.338	0.515244	0.534119
1.208	0.572102	0.553833	1.274	0.543102	0.544824	1.340	0.514379	0.533750
1.210	0.571221	0.553588	1.276	0.542227	0.544515	1.342	0.513515	0.533388
1.212	0.570340	0.553352	1.278	0.541351	0.544209	1.344	0.512651	0.533020
1.214	0.569460	0.553105	1.280	0.540476	0.543896	1.346	0.511788	0.532658
1.216	0.568579	0.552854	1.282	0.539602	0.543589	1.348	0.510925	0.532283
1.218	0.567698	0.552611	1.284	0.538728	0.543269	1.350	0.510063	0.531915
1.220	0.566817	0.552358	1.286	0.537854	0.542959	1.352	0.509201	0.531543
1.222	0.565937	0.552109	1.288	0.536980	0.542638	1.354	0.508339	0.531169
1.224	0.565057	0.551851	1.290	0.536106	0.542315	1.356	0.507478	0.530791
1.226	0.564176	0.551600	1.292	0.535233	0.541993	1.358	0.506617	0.530416
1.228	0.563296	0.551339	1.294	0.534360	0.541670	1.360	0.505757	0.530035
1.230	0.562416	0.551078	1.296	0.533488	0.541348	1.362	0.504897	0.529661
1.232	0.561537	0.550815	1.298	0.532616	0.541018	1.364	0.504038	0.529276
1.234	0.560657	0.550553	1.300	0.531744	0.540692	1.366	0.503179	0.528893
						1.368	0.502321	0.528509

TABLE XX. : BASIC OVERLAP INTEGRALS FOR HYDROGEN-CARBON BONDS

R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)
1.050	0.592103	0.510396	1.083	0.575139	0.506063	1.116	0.558268	0.501062
1.051	0.591588	0.510275	1.084	0.574626	0.505921	1.117	0.557759	0.500901
1.052	0.591073	0.510153	1.085	0.574114	0.505779	1.118	0.557250	0.500739
1.053	0.590558	0.510031	1.086	0.573601	0.505635	1.119	0.556740	0.500576
1.054	0.590043	0.509908	1.087	0.573088	0.505491	1.120	0.556231	0.500413
1.055	0.589528	0.509785	1.088	0.572576	0.505347	1.121	0.555723	0.500250
1.056	0.589013	0.509660	1.089	0.572064	0.505202	1.122	0.555214	0.500086
1.057	0.588499	0.509536	1.090	0.571551	0.505056	1.123	0.554705	0.499921
1.058	0.587984	0.509410	1.091	0.571039	0.504910	1.124	0.554196	0.499756
1.059	0.587470	0.509284	1.092	0.570527	0.504763	1.125	0.553688	0.499590
1.060	0.586955	0.509157	1.093	0.570015	0.504616	1.126	0.553179	0.499423
1.061	0.586440	0.509030	1.094	0.569503	0.504468	1.127	0.552671	0.499257
1.062	0.585926	0.508901	1.095	0.568992	0.504319	1.128	0.552163	0.499089
1.063	0.585411	0.508773	1.096	0.568480	0.504170	1.129	0.551655	0.498921
1.064	0.584897	0.508643	1.097	0.567969	0.504020	1.130	0.551147	0.498753
1.065	0.584383	0.508513	1.098	0.567457	0.503869	1.131	0.550640	0.498583
1.066	0.583869	0.508382	1.099	0.566946	0.503718	1.132	0.550132	0.498414
1.067	0.583355	0.508251	1.100	0.566434	0.503567	1.133	0.549625	0.498244
1.068	0.582841	0.508119	1.101	0.565923	0.503415	1.134	0.549117	0.498073
1.069	0.582327	0.507986	1.102	0.565412	0.503262	1.135	0.548610	0.497902
1.070	0.581813	0.507853	1.103	0.564901	0.503108	1.136	0.548103	0.497730
1.071	0.581299	0.507719	1.104	0.564390	0.502954	1.137	0.547596	0.497558
1.072	0.580785	0.507585	1.105	0.563880	0.502800	1.138	0.547089	0.497385
1.073	0.580272	0.507449	1.106	0.563369	0.502645	1.139	0.546583	0.497211
1.074	0.579758	0.507313	1.107	0.562858	0.502489	1.140	0.546076	0.497037
1.075	0.579244	0.507177	1.108	0.562348	0.502333	1.141	0.545570	0.496863
1.076	0.578731	0.507040	1.109	0.561838	0.502176	1.142	0.545063	0.496688
1.077	0.578218	0.506902	1.110	0.561327	0.502019	1.143	0.544557	0.496513
1.078	0.577704	0.506764	1.111	0.560817	0.501861	1.144	0.544051	0.496337
1.079	0.577191	0.506625	1.112	0.560307	0.501702	1.145	0.543546	0.496160
1.080	0.576678	0.506485	1.113	0.559797	0.501543	1.146	0.543040	0.495983
1.081	0.576165	0.506345	1.114	0.559288	0.501383	1.147	0.542534	0.495806
1.082	0.575652	0.506205	1.115	0.558778	0.501223	1.148	0.542029	0.495623
						1.149	0.541524	0.495449

TABLE XXI : BASIC OVERLAP INTEGRALS FOR HYDROGEN-NITROGEN BONDS

R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)
0.970	0.576154	0.456858	1.004	0.557233	0.451833	1.038	0.538495	0.446091
0.972	0.575037	0.456583	1.006	0.556125	0.451514	1.040	0.537400	0.445733
0.974	0.573920	0.456306	1.008	0.555018	0.451193	1.042	0.536305	0.445372
0.976	0.572804	0.456026	1.010	0.553912	0.450869	1.044	0.535211	0.445009
0.978	0.571688	0.455744	1.012	0.552806	0.450543	1.046	0.534118	0.444644
0.980	0.570572	0.455458	1.014	0.551701	0.450215	1.048	0.533025	0.444277
0.982	0.569458	0.455170	1.016	0.550596	0.449884	1.050	0.531934	0.443907
0.984	0.568343	0.454880	1.018	0.549493	0.449551	1.052	0.530843	0.443536
0.986	0.567230	0.454587	1.020	0.548390	0.449216	1.054	0.529753	0.443162
0.988	0.566117	0.454291	1.022	0.547287	0.448878	1.056	0.528664	0.442786
0.990	0.565004	0.453993	1.024	0.546186	0.448537	1.058	0.527576	0.442408
0.992	0.563892	0.453692	1.026	0.545085	0.448195	1.060	0.526488	0.442028
0.994	0.562781	0.453388	1.028	0.543985	0.447850	1.062	0.525402	0.441646
0.996	0.561670	0.453082	1.030	0.542885	0.447503	1.064	0.524316	0.441262
0.998	0.560560	0.452773	1.032	0.541787	0.447153	1.066	0.523231	0.440876
1.000	0.559450	0.452462	1.034	0.540689	0.446802	1.068	0.522147	0.440488
1.002	0.558341	0.452149	1.036	0.539592	0.446447			

TABLE XXII. : BASIC OVERLAP INTEGRALS FOR HYDROGEN-OXYGEN BONDS

R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)
0.930	0.538109	0.415134	0.963	0.519157	0.410013	0.996	0.500476	0.404255
0.931	0.537531	0.414989	0.964	0.518587	0.409848	0.997	0.499915	0.404071
0.932	0.536953	0.414843	0.965	0.518017	0.409682	0.998	0.499353	0.403887
0.933	0.536376	0.414697	0.966	0.517447	0.409515	0.999	0.498793	0.403702
0.934	0.535798	0.414550	0.967	0.516878	0.409348	1.000	0.498232	0.403517
0.935	0.535221	0.414402	0.968	0.516309	0.409180	1.001	0.497672	0.403331
0.936	0.534645	0.414254	0.969	0.515739	0.409012	1.002	0.497111	0.403145
0.937	0.534068	0.414105	0.970	0.515171	0.408843	1.003	0.496552	0.402958
0.938	0.533492	0.413955	0.971	0.514602	0.408673	1.004	0.495992	0.402771
0.939	0.532916	0.413805	0.972	0.514034	0.408503	1.005	0.495433	0.402583
0.940	0.532340	0.413654	0.973	0.513466	0.408333	1.006	0.494874	0.402394
0.941	0.531764	0.413502	0.974	0.512898	0.408161	1.007	0.494315	0.402206
0.942	0.531188	0.413350	0.975	0.512331	0.407990	1.008	0.493757	0.402016
0.943	0.530613	0.413198	0.976	0.511764	0.407817	1.009	0.493199	0.401826
0.944	0.530038	0.413044	0.977	0.511197	0.407644	1.010	0.492641	0.401636
0.945	0.529463	0.412890	0.978	0.510630	0.407471	1.011	0.492084	0.401445
0.946	0.528889	0.412735	0.979	0.510064	0.407297	1.012	0.491527	0.401254
0.947	0.528314	0.412580	0.980	0.509498	0.407122	1.013	0.490970	0.401062
0.948	0.527740	0.412424	0.981	0.508932	0.406947	1.014	0.490413	0.400870
0.949	0.527166	0.412268	0.982	0.508366	0.406771	1.015	0.489857	0.400677
0.950	0.526593	0.412111	0.983	0.507801	0.406595	1.016	0.489301	0.400484
0.951	0.526019	0.411953	0.984	0.507236	0.406418	1.017	0.488745	0.400290
0.952	0.525446	0.411795	0.985	0.506671	0.406241	1.018	0.488190	0.400095
0.953	0.524873	0.411636	0.986	0.506106	0.406063	1.019	0.487635	0.399901
0.954	0.524301	0.411476	0.987	0.505542	0.405885	1.020	0.487080	0.399705
0.955	0.523728	0.411316	0.988	0.504978	0.405706	1.021	0.486526	0.399510
0.956	0.523156	0.411155	0.989	0.504414	0.405526	1.022	0.485971	0.399314
0.957	0.522584	0.410994	0.990	0.503851	0.405346	1,023	0.485417	0.399117
0.958	0.522012	0.410832	0.991	0.503288	0.405166	1.024	0.484864	0.398920
0.959	0.521441	0.410669	0.992	0.502725	0.404984	1.025	0.484311	0.398722
0.960	0.520869	0.410506	0.993	0.502162	0.404803	1.026	0.483758	0.398524
0.961	0.520299	0.410343	0.994	0.501600	0.404621	1.027	0.483205	0.398325
0.962	0.519728	0.410178	0.995	0.501038	0.404438	1.028	0.482653	0.398126
						1.029	0.482101	0.397927

TABLE XXIII. : BASIC OVERLAP INTEGRALS FOR HYDROGEN-FLUORINE BONDS

R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)
0.900	0.498759	0.372522	0.906	0.495281	0.371577	0.912	0.491813	0.370611
0.901	0.498179	0.372366	0.907	0.494702	0.371417	0.913	0.491236	0.370448
0.902	0.497599	0.372209	0.908	0.494124	0.371257	0.914	0.490659	0.370284
0.903	0.497019	0.372052	0.909	0.493545	0.371096	0.915	0.490083	0.370120
0.904	0.496439	0.371894	0.910	0.492968	0.370935	0.916	0.489507	0.369955
0.905	0.495860	0.371736	0.911	0.492390	0.370773	0.917	0.488931	0.369790

Continued on next page.

TABLE XXIII. : BASIC OVERLAP INTEGRALS FOR HYDROGEN-FLUORINE BONDS (CONTINUED)

R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)	R	(1s,2s)	(1s,2p)
0.918	0.488356	0.369624	0.926	0.483763	0.368276	0.934	0.479191	0.366894
0.919	0.487780	0.369457	0.927	0.483190	0.368106	0.935	0.478621	0.366719
0.920	0.487205	0.369290	0.928	0.482618	0.367934	0.936	0.478051	0.366543
0.921	0.486631	0.369123	0.929	0.482046	0.367762	0.937	0.477481	0.366367
0.922	0.486057	0.368955	0.930	0.481474	0.367590	0.938	0.476912	0.366190
0.923	0.485483	0.368786	0.931	0.480903	0.367416	0.939	0.476344	0.366013
0.924	0.484909	0.368617	0.932	0.480332	0.367243	0.940	0.475775	0.365835
0.925	0.484336	0.368447	0.933	0.479761	0.367069			

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IZVOD

Tabele integrala prekrivanja

L. Klasinc, D. Schulte-Frohlinde i M. Randić

U radu su dane tabele integrala prekrivanja za veze koje čine slijedeći atomi prve periode sistema elemenata: B, C, N, O, F, kao i za veze koje čine isti sa vodikom. Za formu atomskih orbitala uzete su funkcije koje je preporučio za molekularna izračunavanja Clementi. Interval međuatomskih razmaka (dužina veza) koji je tabeliran, odabran je tako da pokriva sve poznate dužine veza gornjih atoma koje srećemo u literaturi.

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Note

Susceptibility Measurements and ^{19}F Chemical Shift of Platinum Hexafluoride

J. Zupan, E. Pirkmajer, and J. Slivnik

Nuclear Institute »J. Stefan«, Ljubljana, Slovenia, Yugoslavia

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Platinum hexafluoride was prepared by pressure synthesis in our laboratory[1], filled in a glass capillary and stored in liquid nitrogen. The susceptibility measurements were made in the range from 170° to 300° K by Gouy's method using $HgCo(SCN)_4$ as standard[2]. As an independent check, with the same standard, the magnetic susceptibility of osmium hexafluoride was also determined. The values obtained are in fair agreement with the values determined by Hargreaves and Peacock[3].

The data collected in Table I yield $\chi_M = (8.13 \pm 0.20) \times 10^{-4}$ c. g. s. units for the *temperature independent* paramagnetism of PtF_6 (after correcting for diamagnetism by $\chi_{dia} = -88 \times 10^{-6}$ c. g. s. units[4]).

TABLE I

Temperature (°K)	170	186	201	216	231	246	259	273	294
$X_g \times 10^6$ (c. g. s. u.)	2.38	2.30	2.31	2.39	2.33	2.33	2.38	2.39	2.33
$X_M \times 10^4$ (c. g. s. u.)	8.23	8.01	8.03	8.26	0.08	8.07	8.23	8.26	8.08

This finding is in agreement with the theoretical prediction by Moffitt, Goodman, Fred and Weinstock[5]. Further confirmation of this was obtained by observing also from 150° to 273° K a *temperature independent* fluorine NMR chemical shift of 4400 ± 200 p. p. m. relative to HF.

Magnetic properties of some other hexafluorides are being investigated.

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IZVLEČEK

Merjenje magnetne susceptibilnosti in kemičnega premika ^{19}F v platinovem heksafluoridu

J. Zupan, E. Pirkmajer in J. Slivnik

Merili smo magnetno susceptibilnost platinovega heksafluorida po Gouyjevi metodi. Ugotovili smo, da se temperaturno neodvisni paramagnetizem ujema tako s teoretičnimi predvidevanji, kot z merjenjem magnetne resonance ^{19}F. Ponovili smo merjenje magnetne susceptibilnosti osmijevega heksafluorida in primerjali rezultate z objavljenimi.

NUKLEARNI INŠTITUT »JOŽEF STEFAN«,
LJUBLJANA

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