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Note

Extension of GAUSSIAN70 to Any Number of Atomic Orbitals

The ab initio molecular orbital calculation program GAUSSIAN70 has recently been released to the scientific community [1] and will undoubtedly be widely used much as CNINDO was some years earlier [2]. It is currently restricted to 80 shells, 6 gaussians per shell (240 maximum), 35 atoms and 70 atomic orbitals (AOs). All of these except the last may be extended by simple changes to the program.

Many highly interesting molecules require more than 70 AOs; however, computational requirements (storage and time) increase rapidly as the number of AOs rises. For maximum utility it is essential that the user be able to tailor program size to the size of molecule to be studied. Changing the number of AOs necessitates modification of the program beyond simple redimensioning. File structure and allocation must be carefully varied to conform to the new requirements.

A general method for the extension of GAUSSIAN70 to any number of AOs is given below (Pullman [3] has recently indicated extension to 105 AOs without details). A 99 orbital version has been successfully used in our laboratories to examine some biologically active molecules [4]. The method presented will allow the prospective user to modify the program to the task at hand without incurring the high initial programming time cost needed to determine the appropriate changes.

Three basic changes need to be made to the program as it is received from QCPE (all card numbers refer to the QCPE deck). First, the dimensions of several arrays must be modified. Second, the DATA statement in subroutine TWRITE must be changed. Last, the allocation of 82 files of 1800 single precision (900 double precision) words each must be increased. In the example below, modification to 99 atomic orbitals (AOs) will be illustrated.

Changes needed to redimension the program are shown in Table I. All new dimensions can be calculated from the equations below, given N (the desired numbers of AOs).

$$A = N + 1, \tag{1}$$
$$B = 2*N, \tag{2}$$
$$C = N*(N + 1), \tag{3}$$
$$D = (N*(N + 1))/2, \tag{4}$$
$$E = ((N*(N + 1))/2) + 1, \tag{5}$$
$$F = ((4*N*(N + 1))/2) - (N + 1). \tag{6}$$

TABLE I

Dimension Constant Changes

Card	Change to	Card	Change to	Card	Change to	Card	Change to
4942	*N*	10794	*N*	11441	*N*	11950	*C*
4949	*N*	10797	*N*	11446	*N*	12033	*D, N*
5009	*N*	10866	*N*	11449	*N*	12039	*N*
5011	*D*	10878	*N*	11458	*N*	12068	*D*
5560	*D*	10986	*N*	11461	*N*	12069	*D*
5561	*D*	11034	*N*	11486	*D, A, F*	12075	*D*
5587	*N*	11055	*N*	11506	*A*	12076	*D*
5589	*D*	11213	*N*	11666	*D*	12122	*D*
5982	*D*	11219	*D*	11671	*D*	12126	*N*
5983	*D*	11245	*D*	11685	*D*	12128	*N*
5984	*D*	11250	*N*	11686	*D*	12129	*N*
6129	*N*	11297	*N*	11687	*D*	12131	*N*
6141	*N*	11301	*N*	11688	*D*	12133	*N*
10221	*N*	11303	*N*	11694	*D*	12135	*N*
10226	*N*	11305	*N*	11695	*D*	12136	*N*
10232	*N*	11307	*N*	11696	*D*	12138	*N*
10235	*N*	11312	*N*	11697	*D*	12142	*D*
10292	*N*	11334	*N*	11774	*D*	12143	*D*
10301	*N*	11337	*N*	11775	*D*	12178	*N*
10395	*N*	11352	*N*	11776	*D*	12181	*E*
10443	*N*	11378	*N*	11777	*D*	12182	*E*
10468	*N*	11383	*D*	11792	*D*	12184	*D*
10469	*N*	11409	*D*	11821	*N*	12212	*D*
10783	*N*	11423	*D*	11869	*D, N*	12213	*D*
10788	*N*	11434	*N*	11909	*D, N*	12240	*D*
12801	*A*	13109	*A*	11930	*C*		
12242	*D*	12694	*C*	13061	*N*	13398	*N*
12247	*N*	12709	*C*	13111	*N, B*	13401	*N*
12259	*N*	12738	*N*	13113	*N*	13405	*N*
12262	*N*	12746	*N*	13114	*N*	13407	*N*
12271	*N*	12748	*N*	13158	*B*	13409	*N*
12274	*N*	12754	*N*	13163	*B*	13412	*N*
12277	*D*	12803	*N, B*	13166	*N*	13414	*N*
12290	*D*	12805	*N*	13168	*N*	13417	*N*
12293	*N*	12847	*B*	13171	*N*	13438	*N*
12296	*N*	12852	*B*	13175	*N*	13445	*N*
12305	*N*	12855	*N*	13177	*N*	13454	*N*
12308	*N*	12857	*N*	13179	*N*	13472	*N*
12310	*D*	12860	*N*	13182	*N*	13528	*N*
12311	*D*	12864	*N*	13184	*N*	13588	*N*

Table continued

TABLE I (*continued*)

12337	*D, F, A*	12866	*N*	13187	*N*
12355	*A*	12868	*N*	13208	*N*
12581	*C*	12871	*N*	13215	*N*
12604	*D*	12873	*N*	13259	*N*
12608	*C*	12876	*N*	13277	*N*
12627	*C*	12897	*N*	13348	*A*
12634	*C*	12904	*N*	13350	*N, B*
12674	*C*	12913	*N*	13352	*N*
12675	*C*	12931	*N*	13353	*N*
12678	*E*	13016	*N*	13388	*B*
12692	*C*	13041	*N*	13393	*B*
12693	*C*	13050	*N*	13396	*N*

The numbers calculated substitute for 71, 140, 4970, 2485, 2486, and 9869, respectively, in the QCPE version of GAUSSIAN70. *N* is substituted for 70 when 70 occurs. This step is also a good place to change *I/O* unit numbers from 5, 6, and 7 to whatever is appropriate (cards 718, 719, 720).

The second step in the extension is the recalculation of the number of files needed to store the extended matrices via subroutine TWRITE. Each file holds 900 double words, so the number of files needed is:

$$\text{Files} = (\text{storage needed}/900) + 1. \tag{7}$$

If the storage requirement is an exact multiple of 900, the constant 1 could be dropped. The number of words required can be calculated from (3) and (4) above and substituted as shown in Table II. The DATA statement consists of the starting point of each set of files; the columns marked 70 and 99 in Table II are the DATA statements for 70 and 99 AOs, respectively.

The final change needed is the modification of the file allocation (card 5) to reflect the increased storage requirements. The current number of files (82) should be changed to a number slightly larger than the total required. In the 99 AO case, any number larger than 145 is adequate. The space allocation for unit 18 should be similarly increased via the job control language.

Unit 19 should also be reallocated, since the number of 2-electron integrals also rises. The space requirement for unit 19 is problem-dependent, so no simple size calculation can be made. We have found that 1000 tracks (on a 2314) is adequate for jobs up to about 85 orbitals.

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TABLE II
TWRITE DATA Statement

NFile	No. words	70	Required # files (70)	99	Required # files (99)
1	47	1	1	1	1
2	298	2	1	2	1
3	6000	3	7	3	7
4	*C*	10	6	10	11
5	*N*	16	1	21	1
6	1441	17	2	22	2
7	328	19	1	24	1
8	*D*	20	3	25	6
9–12	0	4*0	—	4*0	—
13	*D*	23	3	31	6
14	0	0	—	—	—
15	*D*	26	3	37	6
16	0	0	—	0	—
17	*D*	29	3	43	6
18	0	0	—	0	—
19	*D*	32	3	49	6
20	0	0	—	0	—
21	*D*	35	3	55	6
22–24	0	3*0		3*0	—
25	*C*	38	6	61	11
26	0	0	—	0	—
27	*C*	44	6	72	11
28–29	0	2*0	—	2*0	—
30	*C*	50	6	83	11
31	*C*	56	6	94	11
32	*C*	62	6	105	11
33	*C*	68	6	116	11
34	*D*	74	3	127	6
35	*D*	77	3	133	6
36	*D*	80	3	139	6
37–50	0	14*0	—	—	—

REFERENCES

1. Quantum Chemistry Program Exchange #236, QCPE, Indiana University, Bloomington, IN 47401. The program was developed at Carnegie–Mellon University by W. G. Hehre, W. A. Lathan, R. Ditchfield, M. D. Newton, and J. A. Pople. The program uses a sophisticated file handling technique which represents a major advance over past *ab* initio methods.
2. Quantum Chemistry Program Exchange #141, QCPE, Indiana University, Bloomington, IN 47401.
3. G. N. J. PORT AND B. PULLMAN, *Theoret. Chem. Acta* **33** (1974), 275.

4. We have, for example, completed a study on the conformation of hexachlorobenzene, a substance which is implicated in induced porphyria. The essential question is whether the close packing of the Cl's about the benzene ring would lead to a slightly nonplanar array of Cl's. Such does not appear to be the case.

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