To do a sensible refereeing job on this mammoth work was a truly formidable task.

It simply was not possible in the time to check all the formula in detail and it is clearly very important in a work of this kind that such forumulae should be right. It is also the case that they must be printed correctly, so heaven help the printer and the authors when galley proof time comes. It is a sobering thought to remember how many mistakes and misprints there are just in the classic papers in the field. Barnett and Coulson, for example, even manage to get some of their two electron one-centre integrals wrong as the authors will surely know and doubtless take as a dreadful warning!

The job of the referee for such a review is not, of course, to argue with the authors about scientific merit and so on. This is taken for granted and the job of the referee is to "speak for England" in matters of clarity, presentation and balance in the hope of helping the authors to produce a truly classic review. His job is also to pick the "nits" in the manuscript. Some nit-picking has been indicated by pencil marks in the MS, where this seemed appropriate, but before coming to such matters in more detail a general view should be offered.

The authors review that which is widely believed to be a disaster area. Integral-evaluating men, when relaxing and reminiscing, will swap horror stories about what happens when "global" Barnett-Coulson expansion are attempted in many centre calculations.

When such people look at this article they will search through to see how well the authors managed to do one or two of the classic hard cases (3-centre nuclear attraction between high exponent (7 ~ 10), high (n = 2 or 3) principal quantum number orbitals, and similar four centre electron-repulsion integrals). They will not find anything on these and they will not read any further. This will be a pity, but it will happen unless the authors actually give some results on real integrals with accuracy estimates and times.

The only numerical work reported here is in table 2 of Pt. II and the results given in that table (thoroughly indirectly relevant to hard integrals) do little to calm anyones fears about the Barnett-Coulson method.

Looking at the introduction to Pt. I, it is difficult to guess from it that it is all about integrals and it hardly prepares the reader for the very dry (but necessary) section on conventions to come next. A re-write of the introduction could help here. Perhaps leaving out the forward references and de-emphasing the gradients would also help.

To the referee it seems as if the natural order of presentation in this work is as follows:

Pt. I 1 (revised), Pt. I 2, Pt. I 3, 6 and 7 with Pt. II 2, Pt. I 8 with Pt. II 5 and then Pt. II 4. Perhaps Pt. I 4 and 5 and Pt. II 6 should appear in some sort of subordinate role and Pt. II 1 be deleted.

/cont.

If Pt. I 3, 6 and 7 are taken together with Pt. II 2, then all the formal apparatus needed for integral evaluation is together in one place, and some duplication and repeated exposition can be avoided. Pt. I 4 and 5 are not central to this theme (in fact there is only one reference from Pt. I 6 and 7 to Pt. I 5 and none to Pt. I 4). To appreciate Pt. I 6 and 7 it is necessary only to know that rotations can be made, not to know the details of how they are made.

The referee is aware that taking Pt. I 8 and Pt. II 5 together before Pt. II 4 may cause problems because of the example arising from Pt. II 4. There are two points here. A straight integral example would be better. Many readers will not give a fig for gradients until they are convinced about the usual integrals. Even if a straight integral example cannot be provided the example can clearly be dressed up as though it were part of such an integral evaluation and the same points made.

The referee has quite a bit of nit-picking to do in Pt. I 4 and 5 but having made the general point above, there is no need to go further now.

Pt. II 4 should come last as something interesting but not central to the review. An added bonus if you will.

Pt. II 6 is really somewhere else. The referee thinks that Barnett did publish this work as a SSMTG preprint, but cannot trace it. The authors would be doing a public service if they donated a copy of their copy to the BLL preprint library. However, though this is an interesting and fascinating section for the professional, it is not of the essence of integral evaluation. Everyone has his own ideas (largely machine dependent) on how problems like this should be tackled, so this section would be better subordinated somewhat to the main work.

/cont.

Details Pt. I

p.1 Sink, no reference.

p.3 There are later relevant Steinborn papers.

p.4 Line 1. Shavitt actually did the first gaussian transform.

Line 7. "dramatically" seems a bit strong in view of Table 2 Pt II.

Line -3. Sharma 1976 a or b?

p.7 L. 8-9. Where is "elsewhere"? A reference please.

Footnote. The reference to unpublished work dated 1975 here (and elsewhere) is to be deprecated. Make it a proper reference or drop it.

Molecular symmetry is utilised in almost every integral package in existence. See also the work of King and Dupuis and Dacre and Elder.

p.11 Para 2. Very clumsy exposition. Why introduce Γ before $R(n,z)$?

p.12 Last para. Unless the reader happens to know the difference between regular and irregular harmonies, he won't realise that he has encountered the former before, since he has not been told.

p.13 The formulae at the top are pretty mistifying. There is no real help in appendix A either until A23. Why not put this to the body of the text here.

p.19-20 The referee regrets the references to Edmonds here who, as the authors will know, gets most of this sort of thing slightly wrong.

The authors seem to invite similar confusion by attempting to distinguish between R and R_o. This leads to a confused discussion below (4.2) (where reference again to this unpublished work 1975, does not help either).

Why not drop this fictitious distinction, there is just one operator, it all depends on how one looks at it.

p.23 Section 5, l. 1. There is no equation (4.1).

p.23-24 The referee has to confess that this discussion of rotations almost had him confused. If the authors re-read it they will surely agree that it needs re-writing starting from the indupitable result that:

$$R\phi(\underset{\sim}{r}) = \phi(\underset{\sim}{R}^{-1}\underset{\sim}{r}) = \phi'(\underset{\sim}{r})$$

/cont.

for a transformation that maps a point $\underset{\sim}{r} \rightarrow \underset{\approx}{R}\underset{\sim}{r}$.

p.24 Para 2, line 1. That reference again!

p.25 Para 2, line 1. Since n is not defined nor is L defined in relation to n, the term for $R(n,\Theta)$ is not helpful. In view of equation (5.3) it seems to be simply wrong. Or is (5.3) wrong?

p.25 Footnote. Why "sic"? The transgressions of Edmonds are extensively documented in the literature, by Bouten in Nuc. Phys. ~ 1966 and by Wolf in Am. J. Phys. 1969 for example. References would help.

p.25 Equation (5.5a). Why not use $d^{(\ell)}_{m'm}$ as is standard here?

p.27 If the result below (5.9) agrees with Edmonds, should it?

p.29 Equation (6.3a)/or(6.3b) unclear.

p.29 Below (6.1). How can (6.1) be a <u>re</u>-statement of (7.4). The reader has no idea yet what (7.4) is.

p.34 Lines 11-12. There is much work by Silverstone that is relevant here (JCP ~ 1969).

p.38 Para 2, line 3. Table (2) in the referee's MS is empty.

p.38 Last para. In the opinion of the referee to say what the authors say here about quadrature is to misunderstand its nature. To commend a quadrature because it misses or underweights difficult parts of the integrand, is a really perverse thing to do. If what it misses is important then it gives the wrong answers.

The statement that "it assigns very much smaller weighting ..." can be true for some kinds of gaussian quadrature, but it won't be true for all types. What the authors ought to show is that the singularities in the integrals are accurately reflected by the singularities in the kernels (weight functions) for the gaussian quadrature they actually chose. The referee imagines that the statement "the numerical accuracy ... is therefore very much better" can be substantiated by reference to the well-known formula for bounding the error of a gaussian quadrature.

p.51 Et seq. Some examples of the kind of bounds that one gets in practice would be helpful here. The referee is inclined to believe that they are often startlingly lousy.

p.59 Below (A.20). A strange use of "indifferently" here.

As a general comment on this section, the referee really missed a specific example on which to fix his mind. It would have been splendid to see each move illustrated by its relevance say to a 3-centre nuclear attraction integral, with a diffuse s on centre A, a contracted s on centre B and attraction from centre C, so that the relevance of local and global choices became evident. It would also be fascinating to know where the authors would, in practice, choose the evaluation centre in this case.

/cont.

Details Pt. II

p.18 Below (4.7). Check these two lines cf p31 and table 2.

p.18 Line 4. From table 2, the claim "sensationally" for Shanks-Wynn seems much too strong. The transform appears to fail to improve the convergence in the cases of poorest convergence - the success of the transform must surely be judged by its worst performance not by its average performance. Why are there blanks in table 2?

p.19 Below (5.2). Barnett, reference?

p.20 Last line. "tachynomic", is it in OED?

p.21 The references for Barnett, at line 8 or line 13.

p.22 Penultimate line. Check definition of A_n.

p.23 Equation (5.6). Check summation limits in (5.6e), and could not the rather obscure notation be improved here?

p.36 Last para. The authors may be correct (at least for some compilers on some machines) in what they say about addressing in (6.1) but (for many machines commonly available) they claim too much for FORTRAN I/O. Since the comments that they make are heavily machine and compiler dependent they do not seem very helpful really.

p.43 Para. 2. The DO loop activation rules will change in the next FORTRAN standard - indeed many manufacturers have already adopted this standard. Perhaps the comment is therefore inappropriate.

p.46 Last entry before integral in (6.17a)? Shouldn't it be Λ not $\bar{\Lambda}$?

p.58 Table 3, column 1, heading?

p.59 Below (6.43b). Can a table be "pre-tabulated"? (What is it before it is a table?)

p.65 (A.34). This is surely very nasty indeed for small t. It seems unlikely that it could be used successfully in Gauss-Laguerre in this case.

p.70 Above (B.4). Is this not a misuse of "trivium"?

p.78 C17 is attractive and it seems a very sensible thing to use, given the high cpu cost of direct access, so why not?