

Paper 2: Productive skills - Section A

Criterion A: Language

- Does the student demonstrate an ability to use the language effectively and accurately?
- Does the student use spelling, calligraphy (see "Glossary of terms"), vocabulary and grammatical structures correctly and accurately?

Marks	Level descriptor	
0	Language inaccuracies completely obscure communication.	
1	Language inaccuracies often obscure communication.	
2	Language is generally accurate and does not obscure communication.	
3	Language is mostly accurate and communication is clear.	

Criterion B: Message

- Is all the relevant information conveyed?

Marks	Level descriptor	
0	No relevant information has been conveyed.	
1	Some relevant information has been conveyed.	
2	More than half of the relevant information has been conveyed.	
3	All relevant information has been conveyed effectively.	

Criterion C: Format

- Does the format correspond to the task?

Marks	Level descriptor	
0	The format is not appropriate.	
1	The format is appropriate.	

Ib Ab Initio Paper Markscheme

David B. Cook



Ib Ab Initio Paper Markscheme:

Ab Initio Calculations Petr Carsky, Miroslav Urban, 2012-12-06 Until recently quantum chemical ab initio calculations were restricted to atoms and very small molecules. As late as in 1960 Allen and Karo stated: "Almost all of our ab initio experience derives from diatomic LCAO calculations. Now we have found in the literature approximately eighty calculations, three fourths of which are for diatomic molecules. There are approximately twenty ab initio calculations for molecules with more than two atoms, but there is a decided dividing line between the existing diatomic and polyatomic wave functions. Confidence in the satisfactory evaluation of the many-center two-electron integrals is very much less than for the diatomic case. Among the noted twenty calculations, SiH₄ was the largest molecule treated. In most cases a minimal basis set was used and the many-center two-electron integrals were calculated in an approximate way. Under these circumstances the ab initio calculations could hardly provide useful chemical information. It is therefore no wonder that the dominating role in the field of chemical applications was played by semiempirical and empirical methods. The situation changed essentially in the next decade. The problem of many-center integrals was solved; efficient and sophisticated computer programs were developed; basis sets suitable for a given type of problem were suggested; and meanwhile a considerable amount of results has been accumulated which serve as a valuable comparative material. The progress was of course inseparable from the development and availability of computers."

Ab initio calculations, 2018 *Ab initio calculation of the structures and properties of molecules* Clifford E. Dykstra, 1988 **Ab Initio Valence Calculations in Chemistry** David B. Cook, 1974-01-01 **Ab Initio** Donelson Gray McCauley Simon, 1988-01-01

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