COMBINATION DIFFERENCES: VICTIM OF A ”BUM RAP”?

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The problem of correlation in data is considered for spectroscopic difference techniques. In the application of the method of combination differences to diatomic rotational structure with R and P branches only, there is no correlation problem, because each line is used only once in computing the differences. Under best circumstances the combination difference method can match the statistically optimum direct fit method exactly in the more limited goal of estimating the rotational and distortional constants for a given level. The correlation problem arises when a Q branch is added to a combination difference treatment, as it does also in the method of successive differences. Treatment of these cases by correlated least squares can again achieve exact agreement with the direct fit.