An Analysis of the Site-Site Cluster Diagram Series KIPPI DYER, JOHN PERKYNS, B.M. PETTITT, Chemistry Department, University of Houston — The site-site cluster diagram series is examined in terms of the generating series of molecular diagrams. Two results are presented. First, the value of certain of the integrated molecular diagrams are shown to be subject to order of integration, such that, for any finite closure on the site-site distribution functions, some diagrams appear as bridge diagrams within one species labelled pair function while being simple non-bridge diagrams for alternate species labels. This results in inconsistent Kirkwood G factors calculated on different sites for heteronuclear molecules in the proper interaction site integral equation theory. Second, the direct and indirect correlation functions are shown to not be equivalent to the angular average of the molecular direct and indirect correlation functions, respectively.

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