Reverse Monte Carlo model calculations on a-C:H two-component systems

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Abstract

Extensive Reverse Monte Carlo model calculations have been performed for several hydrogenated amorphous carbon systems, for which only one, or at most two, neutron diffraction measurement(s) had been carried out. The possibility of determining the microscopic density of the samples, of estimating the chemical composition of the materials, and of deriving reliable (partial) pair correlation functions from reduced-range ($Q_{max} < 15 Å^{-1}$) structure factors have been investigated in particular. The number density could be determined within 10% in most of the (model) cases, whereas the estimation of the composition proved to be successful only in one of the four cases studied here. It is shown that an evaluation of the partial pair correlation functions for these materials is possible on the basis of limited scattering vector range.

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1. Introduction

i) a-C:H

Amorphous materials have a history of successful technological exploitation extending back more than two decades and in that period our knowledge of their properties has grown steadily. However the materials at the core of this continuing fundamental and technological interest are relatively complex and a large number of important questions concerning their properties remain unanswered. Moreover new materials continue to be generated which open up the range of questions still further. A material that offers a particularly intriguing, and certainly one of the broadest ranges of technological potential is amorphous hydrogenated carbon a-C:H (also referred to as 'diamond-like' carbon) which may be prepared harder, denser and more resistant to chemical attack than any other solid hydrocarbon. These properties, along with optical properties such as the optical gap and refractive index, may be varied by changing the deposition parameters, which has lead to a large number of potential applications [1]. High hydrogen content films (>40at % hydrogen) are of polymeric nature (high sp^3 content, but soft and with low density) and low-hydrogen content films tend to be of graphitic character (soft films consisting of large clusters of sp^2 carbon. It should be noted however that it is possible, under suitable conditions, to produce a low-hydrogen content, hard high density amorphous film [2]). We address ourselves to the central problem of understanding their structure and binding at the atomic level.

The structure giving rise to these useful properties is not yet completely understood, although significant progress has been possible beyond the original models involving clusters of sp^2 carbon linked by sp^3 carbon. The reviews of Robertson [3] and Angus et

al [1] give a fuller account of these and other early models, with Robertson's theoretical modelling having been particularly potent in stimulating a great deal of research world-wide. Within the Robertson model, the hydrogen content is seen to stabilise the sp^3 regions reducing the size of any sp^2 clusters, but at the same time increasing the number of network terminating bonds, leading to a maximum hardness at intermediate hydrogen concentrations. However the unparalleled real space resolution provided by our neutron diffraction data [4] together with complementary experimental data from inelastic neutron scattering [5] and high resolution MAS/NMR [6] , allows us for the first time to attempt to comment in detail on carbon bonding environments within the overall random network and the associated nature of the "decoration" of this network by bonded. Interpretation of the new data [7] does not require heterogeneity on the scale proposed by Robertson, but rather suggests a broadly homogeneous distribution of the possible local environments.

During the past few years, many different forms of amorphous carbon [a-C(:H)] prepared by various PVD/CVD methods have been extensively studied by diffraction [7,8]. As it is extremely difficult to prepare relatively large (~0.5gm) isotopically substituted (i.e. deuterated) samples with identical compositions, the three independent measurements that would be necessary for separating directly the three ppcf's, could not practicably be carried out for the majority of these materials [9]. Since the preparation of a-C:H involves deposition from the gaseous phase onto a substrate at ambient temperature, the resulting samples are usually porous, which makes the macroscopic (bulk) density significantly different from the true density of scattering centres. Additionally, the relatively high concentration of hydrogen can prove problematic during the data analysis stage of a neutron diffraction measurement. (^{1}H has a large cross

section for inelastic scattering, and this fact together with its similar mass to the neutron makes inelasticity effects relatively large. In addition it should be noted that ^{1}H - though not ^{2}H - has a negative scattering length for coherent scattering). It is these difficulties, together with the generic limitation of having only a 1-dimensional data set, that have indicated the need for extensive model studies on a-C:H (see also [10,11]).

ii) RMC

The 1-dimensional nature of diffraction, and other structure-dependent data from amorphous materials necessitates the adoption of a model-dependent analysis and interpretation philosophy. The Reverse Monte Carlo method for generating models has been widely used since its original design [12], and has been applied to a broad spectrum of liquid and amorphous materials problems (and more recently to disorder in crystalline systems). Although it bears comparison with the Rietveld refinement method for crystal structure determination using Bragg diffraction data, RMC is necessarily quite different at the level of the basic algorithm: it is a very general, and therefore flexible, Monte Carlo-based method of structural modelling which is designed to make full use of available diffraction data together with other suitable constraints. Like all approaches, RMC has limitations, which derive both from the way in which the method operates and in the range of experimental data that in practice can be incorporated into the model. An RMC-generated model necessarily remains, in essence, a non-unique description based on an arrangement of atoms which is consistent with available wide-angle diffraction data to within experimental errors.

The essence of the RMC method is that "atoms" in a box are moved until the derived pair distribution function, g(r), or more usually the structure factor, S(Q) matches the experimentally measured curves:

- a box is defined having edge dimensions at least twice the value of r at which statistically significant oscillations in g(r) disappear;
- the box is filled with "atoms" (either at random, or using a simple lattice) to a given number density; for a multicomponent system the correct partial number densities must of course be used;
- this is compared with the experimental S(Q), and the new configuration accepted if the associated χ^2 has been reduced (rejection is subject to a probability function dependent on experimental errors);
- the atoms are then moved at random, and at each stage a $S(Q)_{model}$ is calculated;
- the process is repeated until $S(Q)_{model}$ reproduces experiment to within errors. The process is further iterated until an "ensemble average" of configurations is obtained;
- having established the model, one is then able to study coordination distributions, bond angles, ring/chain statistics etc..

RMC has the following advantages:

- A "real" 3-dimensional model is produced; it is non-parameterised and corresponds to a possible physical structure.
- The model is self-consistent and agrees quantitatively with the available data to within its errors.
- Under suitable circumstances complementary data may be combined (e.g. X-ray and neutron diffraction).
- Constraints derived from prior chemical knowledge may be applied.

- No interatomic potential is required since the model is based directly on the data.
- The principals are quite general, so the method may be modified and developed for other tasks.

Possibly the most useful, and potentially the most interesting, exploitation of the RMC method is its application for multicomponent systems where the number of independent (diffraction) experiments is less than the number of partial pair correlation functions (ppcf's, see [13]). This is the situation that pertains, for instance, when there are no suitable stable isotopes for isotopic substitution neutron diffraction; it is then not possible to derive the ppcf's via traditional, direct methods. It has recently been shown [14] that the RMC method in these cases becomes, not surprisingly, more sensitive to some external parameters, such as the particle sizes. We stress that RMC is not a 'cure-all' method for determining unique solutions from poorly conditioned data. Rather it appears a tractable and efficient method for exploring aspects of the materials' structure by generating models that are always consistent with the full dynamic range of the data available and which may be further constrained by prior knowledge (e.g. by constraints derived from basic chemistry).

More recently it has become apparent that the use of RMC is not limited to 'conventional' structural modelling of diffraction data, but it can also reveal information that the structure factor, S(Q), does contain, but which is not directly accessible. An obvious example is the determination of the microscopic number density (that is, the number density of scattering centres as opposed to the measured macroscopic, or bulk density), which was shown to be obtainable by RMC for a number of different materials [10]. This is an important point, since it is often not possible to determine the

microscopic density directly. The fact that RMC is sensitive to the choice of the number density is, in a sense trivial, since it is s quantity at the heart of all modelling methods; however, what is not trivial is that RMC might consistently yield the *correct* number density, at least if the structure factor is modelled. Another application was the determination of (partial) pair correlation function(s) on the basis of limited Q-space information [11]. This latter approach works primarily because RMC, being an inverse method for determining the pair correlation function, avoids most of the truncation problems that occur when direct Fourier transformation is used. It is therefore better able to isolate information from the S(Q), all sections of which contain information *on all* Fourier components (limited, of course, by the associated experimental errors). This application may prove important when the wide Q range of the most up to date neutron (or X-ray) sources is not available, or when the data at high Q contains large statistical and/or systematic errors. Both in [10] and [11] examples of experimental data were chosen having a sufficient number of independent measurements such that the ppcf's were also calculable via direct separation (i.e. by the direct solution of a set of linear equations by matrix inversion); the effectiveness of the method could thereby be established with more rigour.In this work the possible application of RMC for the above two purposes is investigated for two component systems where the sufficient number of independent experiments for the direct determination of the partials cannot be carried out.

2. Determination of the number density of some model a-C:H samples

The computational studies described here follow the fashion of those presented in [10], i.e. it was verified using model data that the correct number density was indeed

associated with the fit returning the lowest χ^2_{min} value. Details of the model systems considered here are given in Table 1.

As a density search for a multicomponent system has never been carried out before on the basis of only one (or possibly two) structure factor(s), initial investigations were based on the use of model partial structure factors (which were then used as though they were, in fact, total S(Q)s - see CYHE1, PROP1, PROP2, PROP3). The necessary model partial structure factors were obtained from the best RMC fits to real experimental data, i.e. to the experimental S(Q). Density search calculation series for a given model were started from identical initial box configurations, and during the calculations roughly the same number of accepted moves, usually $>10^6$, were completed. As can be seen from Tables 2 and 3, even if only one partial structure factor was used, the correct model density could be found with no difficulty. Note that for finding one single density quite a number of relatively long calculations have to be carried out (this number was usually 5 for our systems). We believe that more precise minima could have been found; however, we have opted for exploring wider density ranges, keeping the quantity of calculations within manageable limits. It was thought to be more important to demonstrate that densities found via RMC are unique, i.e. that there is only one minimum for each system, than to find them more precisely (especially since there does not seem to be any ambiguity, such as an asymmetry of the density - χ^2_{min} curves).

It is apparent from Table 2 that less ideal 'measurements' could be dealt with almost as easily. Closer inspection reveals that the definition of the minimum (that is, the narrowness of the 'curve') does depend on the actual weighting factors adopted (see CYHE3 and CYHE4). It seems that the negative scattering length associated with ^1H

causes the minimum to be more vaguely defined, although for practical purposes the CYHE3 value is almost as good as CYHE4.

3. Composition search

For materials like amorphous hydrogenated silicon-carbon alloys, a-Si:C:H, it is prohibitively difficult to determine with precision the composition of the sample using either chemical or conventional spectroscopic methods [15]; similar problems occur in the case of mixed sol-gel glass systems [16]. In principle, the measured structure factor (or more precisely, the normalised intensity) contains this information inherently, so that RMC might be able to help to estimate the concentrations of the components in an analogous way as it was for density determination.

Four calculation series have been carried out, for model systems described in Table 4. Note that in order to find the composition corresponding to the minimum disagreement between theory and experiment (the smallest χ^2_{min}), separate initial particle configurations had to be generated for each trial composition (and naturally, the weighting factors had to be calculated for them individually as well). For this reason the series could not be standardised as much as it was possible during the density search since no identical initial states were possible. It should also be mentioned that the most problematic systems, from the point of view of their unknown compositions, often have three or more chemical components; hence, a similar search through parameter space to determine them would involve a considerably larger number of RMC calculations.

Our results are summarised in Table 5. As it can be seen, there is usually a minimum value of χ^2 for each series (although these minima are quite shallow), but the minimum is rarely found at the composition determined by standard chemical methods (- in the present case of a-C:H this was by combustion analysis). It is interesting to note that the least meaningful results come from the series where partial, rather than total, structure factors were modelled. This finding might seem to be in contradiction with common sense, but in fact it is not, since if one of the partials totally outweights the others in the total S(Q) (see CYHE5), then by definition the S(Q) contains less information about the other (pairwise) concentrations. (In the CYHE1 case, where there are three partials involved, the situation is perhaps somewhat better.) It must therefore be concluded that using the RMC method for finding an unknown composition is, in general, not applicable. Before applying it for real data, careful model studies have first to be performed in order to test if a given weighting factor combination allows an accurate estimate of the correct composition.

4. Determination of the partial pair correlation functions from reduced range S(Q)'s

As was noted in earlier work [11], only fully determined examples had previously been considered (i.e. where the number of independent measurements is sufficient for the number of partials involved) . Here we investigate whether the partial pair correlation functions could be obtained from limited Q-space information using just one structure factor. The general strategy followed in the present work is in accord with that of [11]: the full structure factor was shortened by 2-3 $Å^{-1}$ at a time, until the partial pair correlation functions, obtained via the Reverse Monte Carlo method on the basis of the

shortened version of the S(Q), have notably deviated from the ones derived on the basis of the full structure factor. (By 'notable deviation' we mean alterations that would be comparable to those associated with truncation effects that occur when direct Fourier transforms are carried out after identical reductions of the Q range. See the case of model amorphous Si in Ref. [11].)

As the separation of the ppcf's on the basis of only one measurement has its own ambiguities (see [13] and [17]), it was of primary importance to make sure that during the process only the effects of shortening the 'experimental' (model) structure factor were to be detected. Two model systems, corresponding in this case to real systems, were applied in the current study: CYHE4 and PROP4. The full model structure factors for both were best RMC fits to the corresponding real systems (see [7,17]). In both cases only the high Q end of the structure factors have been cut gradually (unlike in [11] where the progressive cutting of the low Q data was also studied in the context of different materials). Individual calculations for PROP4, starting from identical initial configurations and completing approximately the same number of accepted moves, have been carried out for model S(Q)s extending up to Q_{max} = 50 (full version), 25, 15, 12 and 7 $Å^{-1}$. For CYHE4, S(Q)s extended up to Q_{max} = 40 (full version), 20, 15, 11 and 7 $Å^{-1}$. The number density for the PROP4 series was 0.160, whereas for the CYHE4 series it was 0.100 $Å^{-3}$, which in both cases may be slightly higher than the real values.

Some of the resulting partial pair correlation functions for the PROP4 series are shown in Figure 1. (Partials that were obtained on the basis of a model S(Q) extending up to 25 $Å^{-1}$ are indistinguishable from the originals.) Apart from the statistical fluctuations, that are due to the rather fine spacing of r (0.02 Å), there are some visible systematic

discrepancies around the first and second peaks of the C-C partial. This is especially apparent when the Q-range of the S(Q) extended up to only 7Å^{-1}, but also for the case Q_{max} = 12 Å^{-1}. The C-H ppcf is also affected in the former case, but the H-H ppcf is largely invariant with respect to decreasing the Q-range. (The H-H partial, on the other hand, is the most affected by statistical noise, due to the smaller number of H atoms in the simulation box. This may hide some effects of the shortened Q-range.) It seems that, in accordance with the expectations, the partial pair correlation functions here are more sensitive to the shrinking of the dynamic range of the structure factor than they were in the fully determined cases (see the example of $Ni_{62}Nb_{38}$ in [11]). However, the general outcome is still rather encouraging: even when there is only one measurement, and that is only up to 7 Å^{-1}, the ppcf's obtained by RMC are still in reasonable agreement with the ones that would be obtainable on the basis of the full Q-range.

There is one more point to add here: if one considers the unfortunate weighting factors of PROP4, burdened by the highly emphasised negative scattering length of H, then the results shown in Figure 1 might seem more than satisfactory. Indeed, similar calculations for CYHE4 provided even better agreement between ppcf's derived on the basis of large and small Q-ranges. (Weighting factors for CYHE4 were calculated via a small rescaling of the Faber-Ziman formalism, and the sample was deuterated, so that no negative scattering length was involved.)

Perhaps the most remarkable result that has come out of the original experimental measurements [7] was that it was possible to distinguish between double (olefinic) and single carbon:carbon bonds, on the basis of an asymmetry observed at the main peak of the (total) pcf. The former has a bondlength of 1.34Å, whereas the latter is 1.52/4Å

long. The ability of the data to reveal this splitting in a quantitative way (the ratio of single:double bonds was determined to be ~2.5:1) was ascribed to the wide dynamic range for diffraction measurements at a pulsed neutron source. It was of interest to check whether this asymmetry of the first peak of the C-C ppcf could be reproduced on the basis of shorter structure factors. Figure 2 shows an enlargement of the C-C ppcf around the first peak. Statistical fluctuations due to the box size tend to mask some features, but the asymmetry on the low-r side of the peak is at least qualitatively revealed for each curve, although its extent varies. It is only the partial obtained on the basis of the S(Q) extending up to 15 $Å^{-1}$ or higher, however, that agrees quantitatively with the original. It is therefore suggested that such fine details can still be detected by RMC on the basis of short structure factors, but for a quantitative analysis and hence definitive statement, a more careful model RMC calculation series and much better model statistics are needed.

5. Conclusions

Some relatively complicated model structure factors, associated with amorphous hydrogenated carbon samples, have been analysed by the Reverse Monte Carlo method. It has been shown that RMC can be applied for the estimation of the microscopic number density, and for evaluating partial radial distribution functions on the basis of limited Q-range information, even when only one (or two) structure factor(s) has(have) been measured for a two-component system. However, the importance of a wide range of model calculations for each individual sample is emphasised. The possibility of using RMC for the estimation of the composition of the sample was also investigated; it was found that RMC was unable to give an accurate estimate.

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Table 1. Some characteristics of the model systems studied during the density search. Names are constructed so that they indicate the precursor gas (CYHE: cyclohexane; PROP: propane). Weighting factors were calculated using the Faber-Ziman formalism (or, in the cases of CYHE2, CYHE3 and CYHE4, a simple rescaled version of it). The correct model densities do not necessarily correspond to the macroscopic densities of real materials.

System /data set	Composition (%C - %H)	Weighting factors (CC-CH-HH partials)	Correct model density ($Å^{-3}$)
CYHE1	75-25	1.0, 0.0, 0.0 0.0, 1.0, 0.0 0.0, 0.0, 1.0	0.100
CYHE2	75-25	1.0, -0.38, 0.04 1.0, 0.67, 0.11	0.100
CYHE3	75-25	1.0, -0.38, 0.04	0.100
CYHE4	75-25	1.0, 0.67, 0.11	0.100
PROP1	68-32	1.0, 0.0, 0.0 0.0, 1.0, 0.0 0.0, 0.0, 1.0	0.160
PROP2	68-32	1.0, 0.0, 0.0 0.0, 1.0, 0.0	0.160
PROP3	68-32	1.0, 0.0, 0.0	0.160

Table 2. χ^2_{min} *vs.* number density for CYHE-systems. (χ^2_{min} is the quantity measuring the deviation of the calculated structure factor from the 'experimental', that is, in our case, from the model S(Q).) The correct number density is 0.100 $Å^{-3}$.

	Minimum χ^2 for the number density (densities are given in $Å^{-3}$)				
Name	0.060	0.080	0.100	0.120	0.140
CYHE1	17.96	5.14	0.47	6.27	16.02
CYHE2	4.22	1.65	0.80	2.1	4.18
CYHE3	3.47	2.01	1.41	2.45	3.6
CYHE4	6.67	2.48	1.01	2.27	4.62

Table 3. χ^2_{min} *vs.* number density for PROP-systems. The correct number density is 0.160 $Å^{-3}$.

	Minimum χ^2 for the number density (densities are given in $Å^{-3}$)				
Name	0.140	0.150	0.160	0.170	0.180
PROP1	5.8	2.01	0.82	1.58	3.63
PROP2	14.46	3.8	0.66	3.4	11.1
PROP3	18.34	5.02	0.57	4.94	16.9

Table 4. Details of model systems used in the composition search.

System/ data set	Correct atomic composition (%C - %H)	Weighting factors (CC-CH-HH partials)	Correct model density ($Å^{-3}$)
CYHE1	75-25	1.0, 0.0, 0.0 0.0, 1.0, 0.0 0.0, 0.0, 1.0	0.100
CYHE3	75-25	1.0, -0.38, 0.04	0.100
CYHE5	75-25	1.0, 0.0, 0.0	0.100
PROP4	68-32	0.3, -0.34, 0.05	0.160

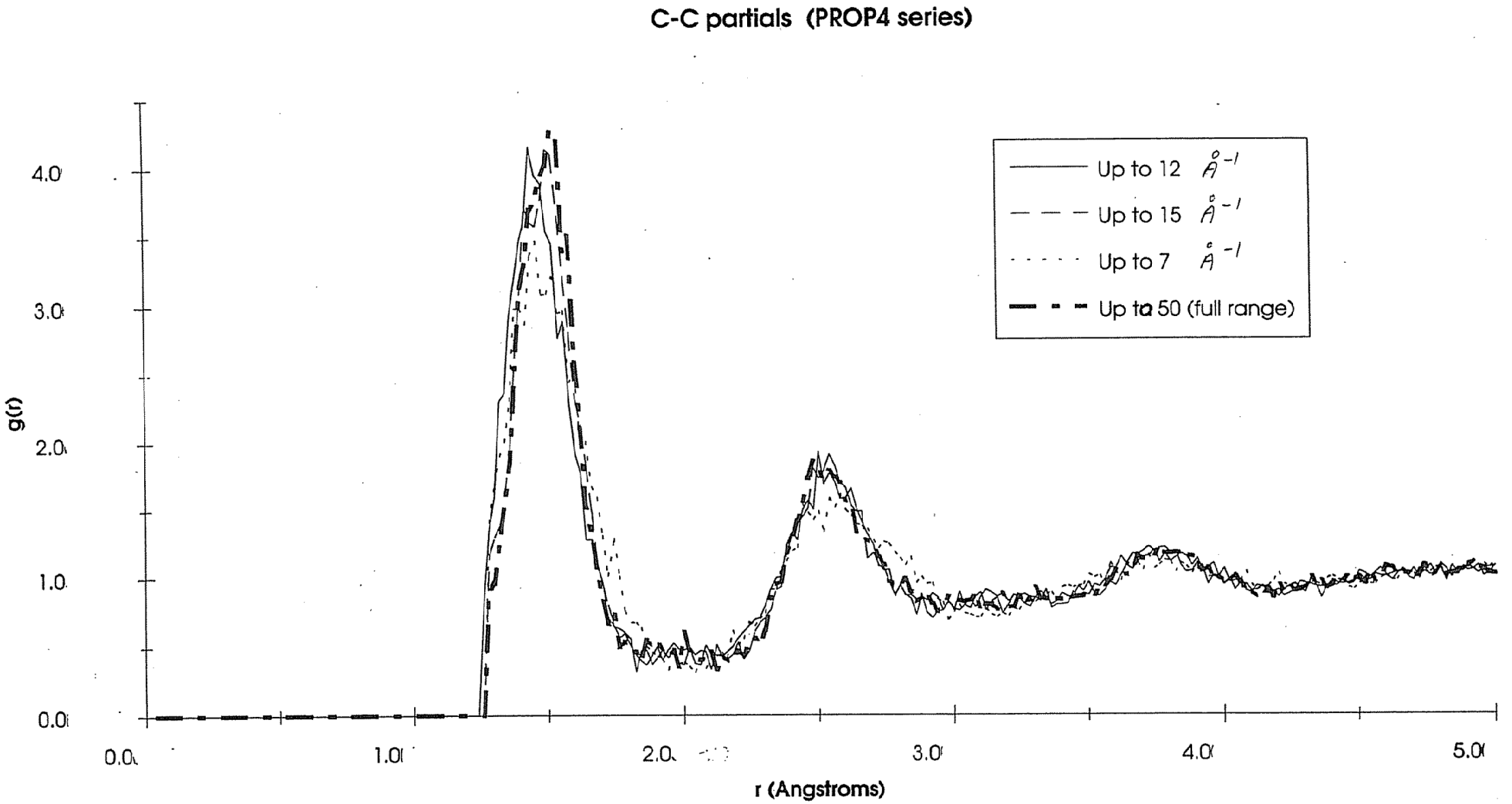
Table 5. χ^2_{min} *vs.* composition data for the composition search. Note that for the CYHE series 68-32 compositions have not been calculated. The correct composition for CYHE systems is 75-25, whereas for the PROP4 system it is 68-32.

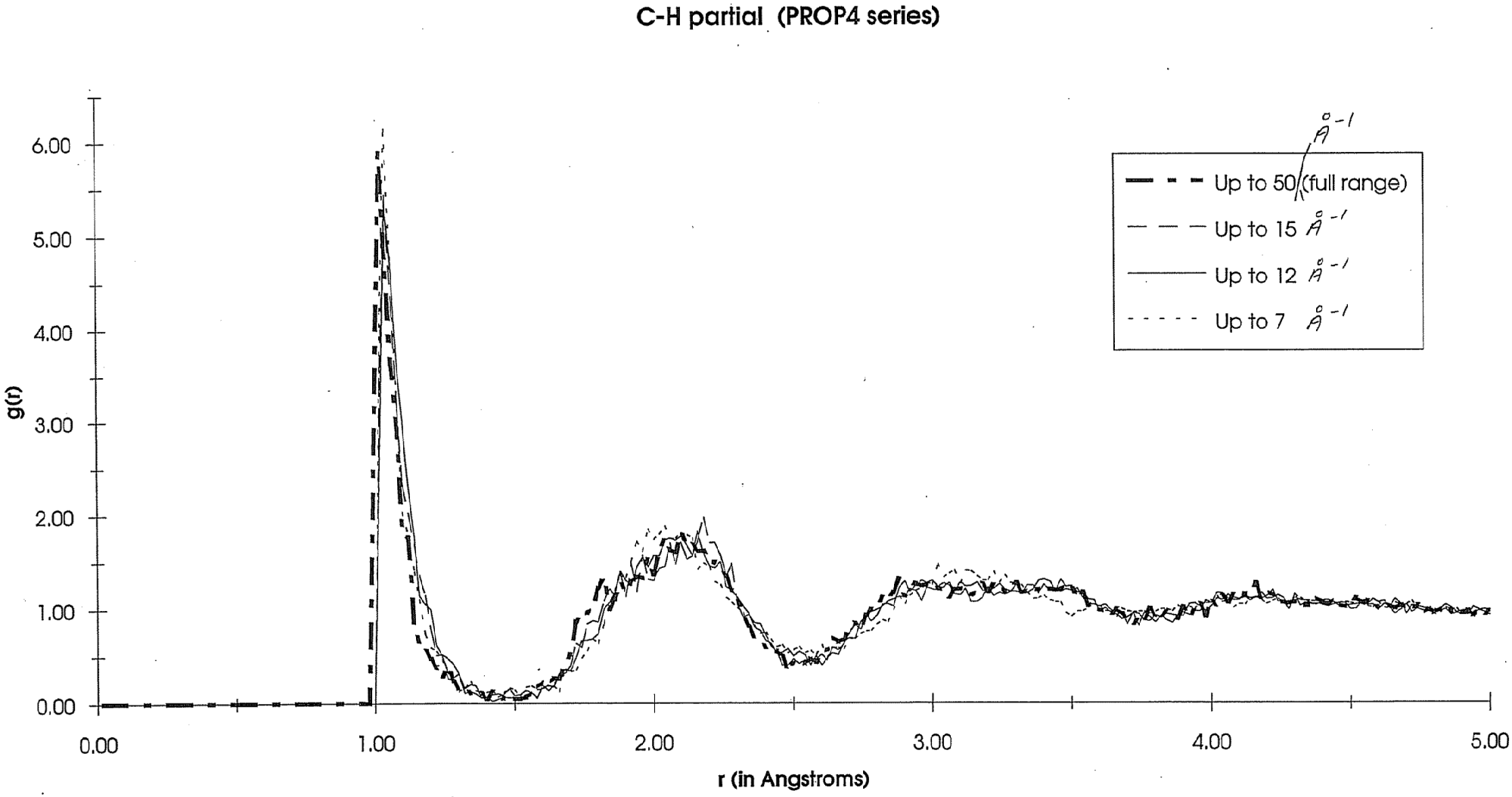
	Minimum χ^2 for the composition (compositions are given in %C-%H)				
Name	50-50	60-40	68-32	75-25	85-15
CYHE1	19.19	9.05	-	4.12	3.97
CYHE3	3.43	1.69	-	2.43	14.19
CYHE5	2.99	3.02	-	3.03	3.12
PROP4	7.43	5.06	4.50	5.02	12.84

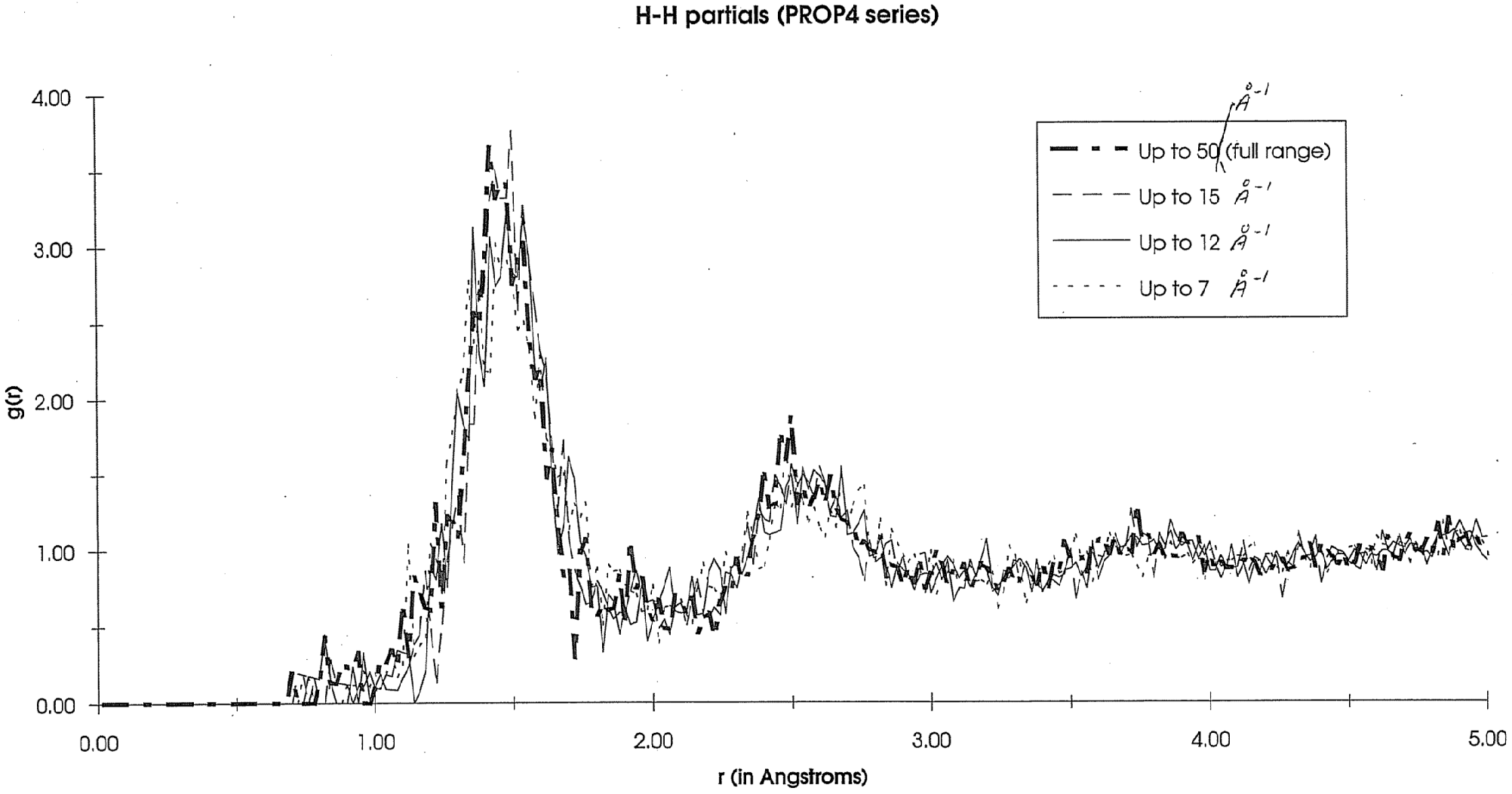
Figure captions

Figure 1. Partial pair correlation functions for the PROP4 series. a) C-C; b) C-H; c) H-H partials.

Figure 2. The C-C partial pair correlation function for the PROP4 series, in the region of the first peak.


C-C partials (PROP4 series)
Up to 12 Å^{-1}
Up to 15 Å^{-1}
Up to 7 Å^{-1}
Up to 50 (full range)
g(r)
4.0
3.0
2.0
1.0
0.0
0.0
1.0
2.0
3.0
4.0
5.0
r (Angstroms)


C-H partial (PROP4 series)
6.00
5.00
4.00
3.00
2.00
1.00
0.00
g(r)
0.00
1.00
2.00
3.00
4.00
5.00
r (in Angstroms)
Up to 50 Å-1 (full range)
Up to 15 Å-1
Up to 12 Å-1
Up to 7 Å-1


H-H partials (PROP4 series)
4.00
3.00
2.00
1.00
0.00
g(r)
0.00
1.00
2.00
3.00
4.00
5.00
r (in Angstroms)
Up to 50 Å-1 (full range)
Up to 15 Å-1
Up to 12 Å-1
Up to 7 Å-1

P.

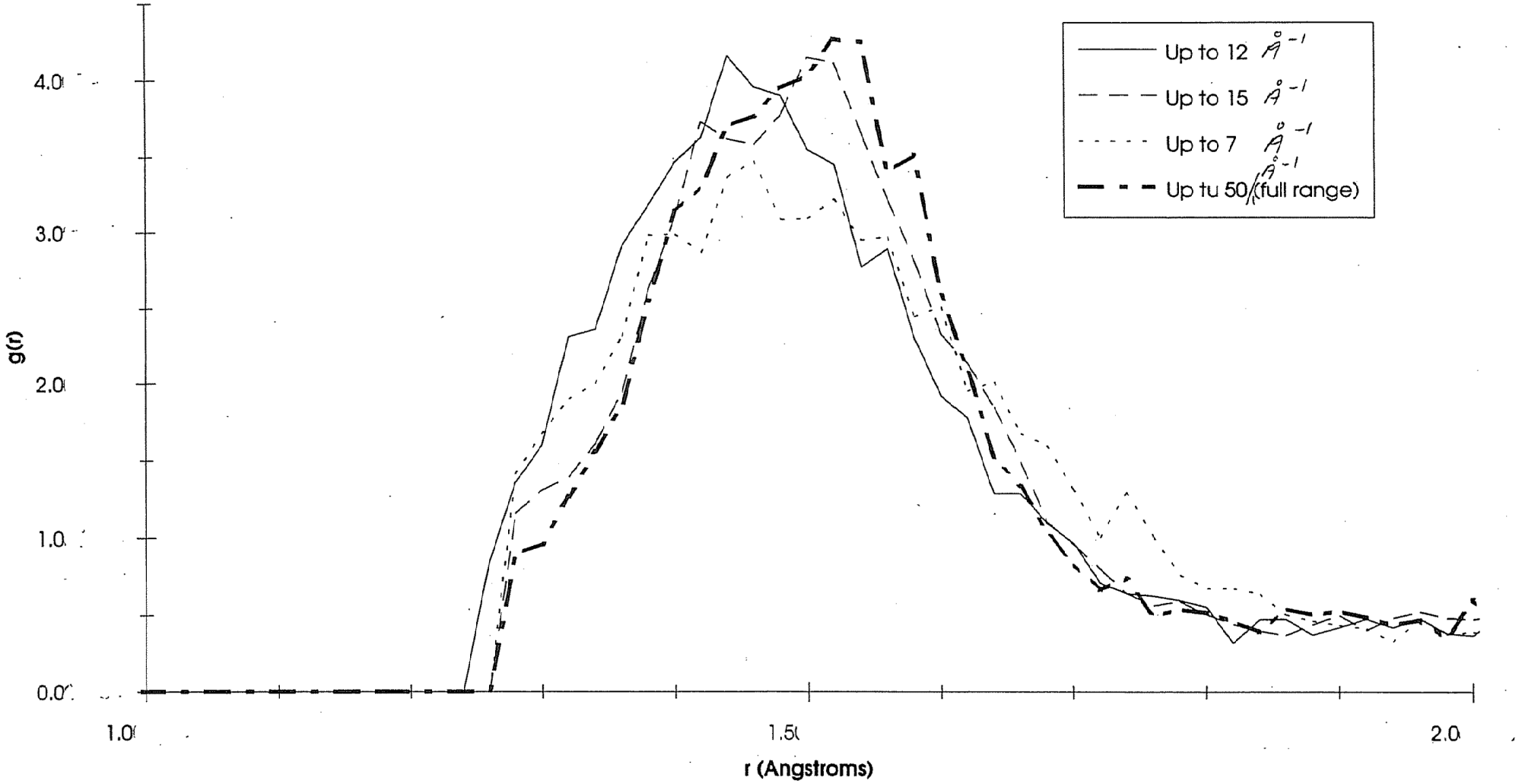

Up to 12 Å⁻¹
Up to 15 Å⁻¹
Up to 7 Å⁻¹
Up tu 50 Å⁻¹ (full range)
g(r)
4.0
3.0
2.0
1.0
0.0
1.0
1.5
2.0
r (Angstroms)

Fig. 1