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# X-ray Scattering and the Chemical Bond in $N_2$ and $CN^-$

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X-ray scattering from the chemical bond within $N_2$ and $CN^-$ has been studied in detail. Differences in scattering from these systems, derived from bonding and non-bonding models, are characterized by *R* values of ~0·04. Partitioning of the scattering into core and valence electron parts clearly demonstrates that the bonding effects are completely situated in the valence electron structure of the systems. Therefore, new evidence has been contributed to support valence structure analysis methods presently employed in X-ray diffraction structure studies.

## Introduction

The molecular form-factor formalism, introduced in a previous paper (Groenewegen & Feil, 1969, henceforth referred to as G & F), resolves the electron density in solid-state structures in terms of molecules instead of atoms. This means that the scattering by a molecule is no longer given by the well known equation

$$f_{\text{molecule}}(\mathbf{s}) = \sum_{\substack{i \text{ atoms in} \\ \text{the molecule}}} f_i \exp(i\mathbf{s}.\mathbf{r}_i) \qquad (1)$$

in which $\mathbf{s}=\mathbf{k}-\mathbf{k}_0$ with $\mathbf{k}_0$ and $\mathbf{k}$ the wave vectors of the incident and scattered beam respectively, $f|_i$ is the atomic form factor and $\mathbf{r}_i$ is the position coordinate with respect to a common origin, of atom *i*. Instead, use is made of the basic equation

$$f(\mathbf{s}) = \langle \psi | \sum_{i=1}^{N} \exp(i\mathbf{s}.\mathbf{r}_i) | \psi \rangle \qquad (2)$$

where $\psi$ is the state function of the *N* electron system of the molecule and $\mathbf{r}_i$ denotes the *i*th position coordinate. In this way bonding effects in the electron distribution are taken care of. Groenewegen & Feil developed and succesfully applied this method to $NH_4F$ to study the chemical bond within the $NH_4^+$ ion. Recently, the topic of the chemical bond in X-ray (and electron) diffraction structure analysis has received considerable attention, and various methods have been proposed and tried to solve the problem (Coppens, 1968; Stewart, 1968, 1969; Bonham, 1969; Harkema & Feil, 1969). This paper presents some new results obtained along the lines developed by G & F. The chemical bond in $N_2$ and $CN^-$ is shown to be observable by X-ray diffraction. A preliminary report on this part has been given elsewhere (Groenewegen, 1969; Zeevalkink, 1970).

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In this paper calculated scattering for $N_2$ and $CN^-$ is partioned into core and valence electron scattering, demonstrating the invariance of core scattering to chemical bonding. These last results support the validity of valence structure methods (Stewart, 1968; Harkema & Feil, 1969) in X-ray diffraction structure analysis.

## Form factors of $N_2$ and $CN^-$

Molecular form factors for coherent X-ray scattering factors are calculated from molecular wave functions, as discussed by G & F. Molecular wave functions of diatomic molecules are usually constructed from a two-centre (TC) basis of Slater type functions or orbitals (STO's). In G & F's paper, where all details of calculating the various scattering integrals were discussed, it was suggested that TC scattering integrals involving STO's are conveniently calculated *via* expansion of the STO's in Gaussian type orbitals (GTO's). A similar approach has been followed by McWeeny (1953) and Stewart (1969). For the present calculations, four term expansions of Huzinaga (1965) and O-ohata, Taketa & Huzinaga (1966) were employed.

Information on the wave functions used to calculate molecular form factors of $N_2$ and $CN^-$ is listed in Table 1. The time required to compute the form factor for a particular value of the scattering vector **s** was 40 seconds on an IBM system 360/50 computer. (This time is relatively long because of the ALGOL programming used.) In the same table, non-bonding isolated atom wave functions are specified. These functions from which non-bonding form factors are derived are simple products of atomic (ionic) wave functions (the product is not antisymmetric as mentioned erroneously in G & F's paper). The corresponding electron density is the sum of the free atomic (ionic) densities properly located. Comparison of the molecular form factors with the non-bonding ones provides information on the scattering from the chemical bond.

Explicit information on bonding and non-bonding form factors of the systems is given in Tables 2 and 3. Because of the axial symmetry the irreducible part of reciprocal **s** space is a quarter plane for $N_2$ and a half plane for $CN^-$. Since $f(-\mathbf{s})=f^*(\mathbf{s})$, a quarter plane suffices for both systems, conveniently limited by some cut-off value of the scattering angles. For the Tables this limit lies near the Cu $K\alpha$ limit. The scattering from the chemical bond, *i.e.* the difference in form factors derived from the molecular wave functions and the corresponding isolated atoms, arrangement, may be appreciable. For **s** parallel to the molecular axis (*i.e.* $s_x=0$) the difference may amount to more than 10% of the total scattering. In accordance with X-ray crystallography practise, we indicate this difference for a group of **s** values by $R$ values which we define in the following way:

Table 1. *Specification of ab initio molecular wave functions for* $N_2$ *and* $CN^-$ *used to calculate form factors*

| | $N_2$ | $CN^-$ |
|---|---|---|
| Reference | Nesbet (1964) | Bonaccorsi, Petrongolo, Scrocc & Tomasio (1968) |
| Approximation | | Self consistent field |
| Type basis | | Double $\zeta+d$ orbitals; STO's |
| State | | ${}^1\Sigma^+_{(g)}$ ground state |
| Interatomic distance | 2·068 a.u. | 2·1791 a.u |
| Calculated energy | −108·97143 a.u. | −92·3233 a.u. |
| Estimated *HF* limit | −108·9888 a.u.<br>(Cade & Sales, 1966) | ? |
| *HF* energy of isolated atoms configuration (Clementi, 1965) | −108·8018 a.u. | $\{C,N^-\}$: −92·0105 a.u.<br>$\{C^-,N\}$: −92·1097 a.u. |

Table 2. *X-ray scattering from* $N_2$ *as a function of the scattering vector* **s**

Upper entries represent the non-bonding form factor $f_{NB}(\mathbf{s})$, while lower entries equal the difference between the non-bonding and the bonding form factor: $\Delta f(\mathbf{s})=f_{NB}(\mathbf{s})-f_B(\mathbf{s})$. Nuclear cartesian coordinates are: (N1): (0,0,0), N(2): (0,0,2·068 a.u.).

| $s_x$ | 0·0 | 0·2 | 0·4 | 0·6 | 0·8 $4\pi$ Å$^{-1}$ |
|---|---|---|---|---|---|
| $s_z$ | | | | | |
| 0·0 $4\pi$ Å$^{-1}$ | $14·00+0·00i$<br>$0·00+0·00i$ | $9·20+0·00i$<br>$-0·10+0·00i$ | $4·80+0·00i$<br>$-0·20+0·00i$ | $3·39+0·00i$<br>$-0·16+0·00i$ | $2·87+0·00i$<br>$-0·10+0·00i$ |
| 0·2 | $0·35+1·75i$<br>$0·02+0·08i$ | $0·26+1·31i$<br>$0·01+0·05i$ | $0·16+0·82i$<br>$0·00+0·01i$ | $0·12+0·63i$<br>$-0·01+0·01i$ | $0·11+0·54i$<br>$0·00-0·01i$ |
| 0·4 | $4·10-1·69i$<br>$0·47-0·20i$ | $3·67-1·52i$<br>$0·29-0·13i$ | $3·02-1·24i$<br>$0·06-0·02i$ | $2·61-1·07i$<br>$-0·01+0·01i$ | $2·32-0·96i$<br>$-0·02+0·00i$ |
| 0·6 | $1·04+1·56i$<br>$0·25+0·22i$ | $1·01+1·51i$<br>$0·11+0·16i$ | $0·93+1·41i$<br>$0·04+0·07i$ | $0·86+1·29i$<br>$0·01+0·02i$ | $0·77+1·16i$ |
| 0·8 | $1·45-1·44i$<br>$0·05-0·05i$ | $1·43-1·42i$<br>$0·05-0·04i$ | $1·36-1·37i$<br>$0·03-0·05i$ | $1·27-1·26i$ | |

Table 3. *X-ray scattering from* $CN^-$ *as a function of the scattering vector* **s**

Upper entries represent non-bonding form factor $f_{NB}(\mathbf{s})$ for the isolated atom $C^-$, N arrangement, while lower entries equal $f_{NB}(\mathbf{s})-f_B(\mathbf{s})$. Nuclear coordinates: N(0,0,0), C(0,0, −2·1791 a.u.). $f_{NB}=f(C^-, N)$

| $s_x$ <br> $s_z$ | 0·0 | 0·2 | 0·4 | 0·6 $4\pi$ Å$^{-1}$ |
|---|---|---|---|---|
| 0·0 $4\pi$ Å$^{-1}$ | 14·00+0·00*i* | 8·19+0·00*i* | 4·34+0·00*i* | 3·23+0·00*i* |
| | 0·00+0·00*i* | −0·36+0·00*i* | −0·19+0·00*i* | −0·12+0·00*i* |
| 0·2 | 1·11−0·86*i* | 0·91−0·63*i* | 0·41−0·43*i* | 0·19−0·36*i* |
| | −0·17−0·09*i* | 0·00+0·00*i* | 0·03+0·03*i* | 0·00+0·02*i* |
| 0·4 | 4·11+0·90*i* | 3·73+0·84*i* | 3·16+0·74*i* | 2·76+0·66*i* |
| | 0·52+0·13*i* | 0·33+0·07*i* | 0·09+0·01*i* | 0·00+0·00*i* |
| 0·6 | 0·55−1·03*i* | 0·53−1·00*i* | 0·48−0·94*i* | 0·45−0·85*i* |
| | 0·07−0·13*i* | 0·06−0·09*i* | 0·02−0·04*i* | 0·00−0·01*i* |
| 0·8 | 2·19+1·09*i* | 2·15+1·07*i* | 2·04+1·01*i* | 1·89+0·92*i* |
| | 0·09+0·03*i* | 0·07+0·03*i* | 0·04+0·02*i* | |

$$R=\sum_{\mathbf{s}} \Delta f(\mathbf{s})/\sum_{\mathbf{s}}|f_B(\mathbf{s})|$$

and

$$R_w=[\sum_{\mathbf{s}}(w\Delta f(\mathbf{s}))^2/\sum(w|f_B(\mathbf{s})|)^2]^{\frac{1}{2}}\,,$$

where $\Delta f(\mathbf{s})=||f_B(\mathbf{s})|-|f_{NB}(\mathbf{s})||$ with $f_B$ the form factor for a set of bonded atoms calculated according to equation (2) and $f_{NB}$ the form factor as calculated in the usual way, [equation (1)], valid for aggregates of non-bonded or isolated atoms. The weighting factor $w$ is given by $w^{-1}=|f_B|$. The summation is over a set of **s** values that corresponds with measurements on $\alpha$-$N_2$ and LiCN which is discussed below. The results for $N_2$ were: $R=0{\cdot}031$, $R_w=0{\cdot}042$ and for $CN^-$: $R=0{\cdot}049$, $R_w=0{\cdot}063$. Tables 2 & 3 show that bond scattering is effectively restricted to $s\le 0{\cdot}8\ 4\pi$Å$^{-1}$.

The results show clearly that the chemical bond is well observable by X-ray diffraction measurements of present-day accuracy.

The results of the comparison of calculated scattering based on bonding and non-bonding models (wave functions) with experiment are shown in Tables 4 and 5. The experimental data employed for this purpose are specified below:

$\alpha$-$N_2$ (Jordan, Smith, Streib & Lipscomb, 1964): single crystal data, Mo $K\alpha$ radiation, $T=25\,°$K; 49 independent reflexions observed (photographically with overlapping films); space group $P2_13$, cubic, 4 molecules/unit cell; $R=\sum||F_{\rm obs}|-|F_{\rm calc}||/\sum|F_{\rm obs}|=0{\cdot}13$; N–N distance $2{\cdot}077\pm0{\cdot}02$ a.u.

LiCN (Lely, 1942): single-crystal data, Cu radiation, room temperature; ±100 independent reflexions observed; space group *Pnma*, orthorhombic, 4 molecules/unit cell; $R\simeq0{\cdot}10$; C–N distance $2{\cdot}16\pm0{\cdot}02$ a.u.

Table 4. *Results of 2-parameter refinement of* $\alpha$-$N_2$ *using isolated atoms* (*IA*) *and molecular* (*M*) *form factors*

*d* is the internuclear distance in a.u. Refined parameters are the overall scale factor (OSF.) and the overall isotropic temperature *B* factor in Å$^2$. Numbers in parentheses indicate standard errors. $R=\sum \Delta F/\sum|F_{\rm obs}|$, $R_w=\{\sum w(\Delta F)^2/\sum w|F_{\rm obs}|^2\}^{1/2}$, $\Delta F=||F_{\rm obs}|-|F_{\rm calc}||$, $w=\sigma_{\rm obs}^{-1}$.

| $N_2$ model | OSF | *B* | *R* | $R_w$ |
|---|---|---|---|---|
| *IA*, *d*=2·077 | 6·70 | 0·59 | 0·136 | 0·138 |
| | (0·25) | (0·21) | | |
| *IA*, *d*=2·068 | 6·69 | 0·56 | 0·135 | 0·137 |
| | (0·25) | (0·20) | | |
| *M*, *d*=2·068 | 6·62 | 0·53 | 0·139 | 0·145 |
| | (0·26) | (0·21) | | |

From the results in Tables 4 & 5, it is seen that the bonding model does not compare better with experiment than a proper non-bonding model does for these structures. The explanation of this inconclusive result may be in (1) the underlying assumptions: LiCN is not purely ionic; what is the effect of libration? (2) the re-

Table 5. *Results of 3-parameter refinement of* LiCN *using isolated atoms* (*IA*) *and molecular* (*M*) *form factors*

Refined parameters are the overall scale factor (OSF) and individual isotropic temperature factor *B* for $Li^+$ and $CN^-$. Double entries below *R* and $R_w$ refer to $\sum$ including observed zero intensities and excluding these respectively. $w=1$.

| $CN^-$ model | | OSF | $B_{Li^+}$ | $B_{CN^-}$ | *R* | $R_w$ |
|---|---|---|---|---|---|---|
| *IA* (C, N), | *d*=2·16 | 1·79 | 4·96 | 5·51 | 0·124 | 0·102 |
| | | (0·03) | (0·47) | (0·23) | 0·096 | 0·094 |
| *IA* ($C^-$, N), | *d*=2·18 | 1·77 | 4·85 | 5·26 | 0·123 | 0·107 |
| | | (0·03) | (0·47) | (0·24) | 0·093 | 0·098 |
| *IA* (C, $N^-$), | *d*=2·18 | 1·76 | 4·90 | 5·16 | 0·113 | 0·090 |
| | | (0·03) | (0·40) | (0·20) | 0·082 | 0·078 |
| *M* $(CN)^-$, | *d*=2·18 | 1·74 | 4·70 | 4·98 | 0·120 | 0·098 |
| | | (0·03) | (0·42) | (0·22) | 0·090 | 0·087 |

finement: *e.g.* in the present work the earlier position parameters have not been reconsidered and (3) the experimental data: the error of measurement ($R \geq 0{\cdot}10$) obscures any fine details like chemical bonding (corresponding to model differences of $R \simeq 0{\cdot}04$, *cf.* above).

### Scattering from core and valence electrons

Since the wave functions used for calculating form factors are all of the SCF type it is a straightforward matter to partition the electron densities involved into core and valence electrons: $\varrho^{\text{core}}$ and $\varrho^{\text{val}}$. Correspondingly, the form factors may be split in core and valence terms: $f = f^{\text{core}} + f^{\text{val}}$. Explicit data on this partitioning of the form factors of $N_2$ and $CN^-$ (themselves listed in Tables 2 and 3) into their core and valence parts are given in Tables 6 to 9. From the Tables it is observed that within the range of scattering vectors (**s**) considered, there is no difference in core electron scattering derived from bonding or non-bonding wave functions! Up to the resolution of observation by X-ray diffraction, core electrons do not participate in chemical bonding. Hence, the observable bonding effects may be ascribed completely to the valence electron structure of the system under investigation.

Table 6. *Core electron scattering from* $N_2$ *as a function of the scattering vector* **s**

Upper entries are $f^{\text{core}}_{NB}(\mathbf{s})$, lower ones give $\Delta f^{\text{core}} = f^{\text{core}}_{NB}(\mathbf{s}) - f^{\text{core}}_{B}(\mathbf{s})$. Nuclear coordinates as in Table 2.

| $s_x$ | 0·0 | 0·2 | 0·4 | 0·6 | 0·8 $4\pi$ Å$^{-1}$ |
|---|---|---|---|---|---|
| $s_z$ | | | | | |
| 0·0 $4\pi$ Å$^{-1}$ | 4·00+0·00*i*<br>0·00+0·00*i* | 3·92+0·00*i*<br>0·00+0·00*i* | 3·69+0·00*i*<br>0·00+0·00*i* | 3·35+0·00*i*<br>0·00+0·00*i* | 2·95+0·00*i*<br>0·00+0·00*i* |
| 0·2 | 0·15+0·75*i*<br>0·00+0·00*i* | 0·15+0·73*i*<br>0·00+0·00*i* | 0·14+0·69*i*<br>0·00+0·00*i* | 0·12+0·63*i*<br>0·00+0·00*i* | 0·11+0·55*i*<br>0·00+0·00*i* |
| 0·4 | 3·15−1·30*i*<br>0·00+0·00*i* | 3·09−1·28*i*<br>0·00+0·00*i* | 2·92−1·20*i*<br>0·00+0·00*i* | 2·66−1·10*i*<br>0·00+0·00*i* | 2·35−0·97*i*<br>0·00+0·00*i* |
| 0·6 | 1·03+1·54*i*<br>0·00+0·00*i* | 1·01+1·52*i*<br>0·00+0·00*i* | 0·95+1·44*i*<br>0·00+0·00*i* | 0·87+1·31*i*<br>0·00+0·00*i* | 0·78+1·17*i* |
| 0·8 | 1·48−1·48*i*<br>0·00+0·00*i* | 1·46−1·45*i*<br>0·00+0·00*i* | 1·39−1·38*i*<br>0·00+0·00*i* | 1·28−1·27*i*<br>0·00+0·00*i* | |

Table 7. *Core electron scattering from* $CN^-$ *as a function of the scattering vector* **s**

Upper entries are $f^{\text{core}}_{NB}(\mathbf{s})$, lower ones give $\Delta f^{\text{core}} = {}^{\text{core}}_{NB}(\mathbf{s}) - f^{\text{core}}_{B}(\mathbf{s})$. Nuclear coordinates as in Table 3. $f_{NB} = f(C^-, N)$.

| $s_x$ | 0·0 | 0·2 | 0·4 | 0·6 $4\pi$ Å$^{-1}$ |
|---|---|---|---|---|
| $s_z$ | | | | |
| 0·0 $4\pi$ Å$^{-1}$ | 4·00+0·00*i*<br>0·00+0·00*i* | 3·90+0·00*i*<br>0·00+0·00*i* | 3·63+0·00*i*<br>0·00+0·00*i* | 3·25+0·00*i*<br>0·00+0·00*i* |
| 0·2 | 0·07−0·47*i*<br>0·00+0·00*i* | 0·09−0·46*i*<br>0·00+0·00*i* | 0·12−0·42*i*<br>0·00+0·00*i* | 0·16−0·37*i*<br>0·00+0·00*i* |
| 0·4 | 3·43+0·84*i*<br>0·00+0·00*i* | 3·35+0·82*i*<br>0·00+0·00*i* | 3·13+0·75*i*<br>0·00+0·00*i* | 2·82+0·67*i*<br>0·00+0·00*i* |
| 0·6 | 0·50−1·05*i*<br>0·00+0·00*i* | 0·50−1·02*i*<br>0·00+0·00*i* | 0·49−0·95*i*<br>0·00+0·00*i* | 0·48−0·85*i*<br>0·00+0·00*i* |
| 0·8 | 2·22+1·10*i*<br>0·00+0·00*i* | 2·18+1·07*i*<br>0·00+0·00*i* | 2·06+1·00*i*<br>0·00+0·00*i* | 1·88+0·90*i*<br>0·00+0·00*i* |

Table 8. *Valence electron scattering from* $N_2$ *as a function of the scattering vector* **s**

Upper entries are $f^{\text{val}}_{NB}$ (s), lower ones give $\triangle f^{\text{val}} = f^{\text{val}}_{NB}(\mathbf{s}) - f^{\text{val}}_{B}(\mathbf{s})$. Nuclear coordinates as in Table 2.

| $s_x$ | 0·0 | 0·2 | 0·4 | 0·6 | 0·8 $4\pi$ Å$^{-1}$ |
|---|---|---|---|---|---|
| $s_z$ | | | | | |
| 0·0 $4\pi$ Å$^{-1}$ | 10·00+0·00*i*<br>0·00+0·00*i* | 5·28+0·00*i*<br>−0·10+0·00*i* | 1·11+0·00*i*<br>−0·20+0·00*i* | 0·04+0·00*i*<br>−0·16+0·00*i* | −0·06+0·00*i*<br>−0·10+0·00*i* |
| 0·2 | 0·20+1·01*i*<br>0·02+0·08*i* | 0·11+0·58*i*<br>0·01+0·05*i* | 0·03+0·13*i*<br>0·00+0·01*i* | 0·00+0·00*i*<br>−0·01−0·01*i* | 0·00−0·01*i*<br>0·00−0·01*i* |
| 0·4 | 0·95−0·39*i*<br>0·47−0·20*i* | 0·58−0·24*i*<br>0·29−0·13*i* | 0·10−0·04*i*<br>0·06−0·20*i* | −0·05+0·02*i*<br>−0·01+0·01*i* | −0·04+0·01*i*<br>−0·02+0·00*i* |
| 0·6 | 0·01+0·02*i*<br>0·25+0·22*i* | 0·00+0·00*i*<br>0·11+0·16*i* | −0·02−0·03*i*<br>0·04+0·07*i* | −0·02−0·03*i*<br>0·01+0·02*i* | 0·00+0·00*i* |
| 0·8 | −0·03+0·03*i*<br>0·05−0·05*i* | −0·03+0·03*i*<br>0·05−0·04*i* | −0·02+0·02*i*<br>0·03−0·05*i* | −0·01+0·01*i* | |

Table 9. *Valence electron scattering from* $CN^-$ *as a function of the scattering vector* **s**

Upper entries are $f_{NB}^{val}(s)$, lower ones give $\Delta f^{val}=f_{NB}^{val}(s)-f_{B}^{val}(s)$. Nuclear coordinates as in Table 3. $f_{NB}=f(C^-, N)$.

| $s_x$ | 0·0 | 0·2 | 0·4 | 0·6 $4\pi$ Å$^{-1}$ |
|---|---|---|---|---|
| $s_z$ | | | | |
| 0·0 $4\pi$ Å$^{-1}$ | 10·00+0·00*i* | 4·29+0·00*i* | 0·70+0·00*i* | −0·01+0·00*i* |
| | 0·00+0·00*i* | −0·36+0·00*i* | −0·19+0·00*i* | −0·12+0·00*i* |
| 0·2 | 1·04−0·40*i* | 0·82−0·17*i* | 0·29−0·01*i* | 0·03+0·01*i* |
| | −0·17−0·09*i* | 0·00+0·00*i* | 0·03+0·03*i* | 0·00+0·02*i* |
| 0·4 | 0·68+0·07*i* | 0·38+0·02*i* | 0·03−0·01*i* | −0·05−0·01*i* |
| | 0·52+0·13*i* | 0·33+0·07*i* | 0·09+0·01*i* | 0·00+0·00*i* |
| 0·6 | 0·05+0·02*i* | 0·02+0·02*i* | −0·01+0·01*i* | −0·03+0·00*i* |
| | 0·07−0·13*i* | 0·06−0·09*i* | 0·02−0·04*i* | 0·00−0·01*i* |
| 0·8 | −0·04−0·01*i* | −0·03+0·00*i* | −0·02+0·01*i* | 0·00+0·01*i* |
| | 0·09+0·03*i* | 0·07+0·03*i* | 0·04+0·02*i* | |

This important observation supports valence structure diffraction analysis techniques as applied by Stewart (1968) and Harkema & Feil (1969). Tables 8 and 9 show further that, compared to $f^{val}$, bonding effects characterized by $\Delta f=\Delta f^{val}$ may be of considerable magnitude.

A similar analysis has been applied to the G & F from factor of $NH_4^+$. Since the irreducible part of reciprocal space here no longer is a plane, these data do not lend themselves for tabulation. The results of the analysis above, however, are completely confirmed also for this system.

## Summary

Molecular form factors of $N_2$ and $CN^-$ calculated from *ab initio* molecular wave functions demonstrate the observability of the chemical bond by X-ray diffraction experiments. Comparison with experimental data on $\alpha$-$N_2$ and LiCN remains inconclusive because of the poor quality of the data. Partitioning of the calculated scattering into core and valence electron parts shows Stewart's assumption on the invariance of core electron scattering to chemical bonding to be correct.

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