

Structure and bonding of ScCN and ScNC: Ground and low-lying states

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ABSTRACT

We have studied the experimentally unknown Sc[CN] molecular system in both its isomeric forms, scandium cyanide (ScCN) and isocyanide (ScNC), through *ab initio* computations. We report energetics, geometries, harmonic frequencies, and dipole moments for the first 20 Sc[CN] states correlating diabatically to $\text{Sc}^+(\text{}^3\text{D}, \text{}^1\text{D}, \text{}^3\text{F}) + \text{CN}^-(\text{}^X \text{}^1\Sigma^+)$. Both isomers have a pronounced ionic character around equilibrium due to the high electron affinity of the CN group and the low ionization energy of the Sc atom. According to our calculations the ScNC isomer ($\text{}^X\text{}^3\Delta$) is stabler than the ScCN($\text{}^X\text{}^3\Delta$) by ~ 5 kcal/mol.

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1. Introduction

The cyano radical $\text{CN}(\text{}^X\text{}^2\Sigma^+)$ belongs to an interesting class of ligands with an ability to form energetically close isomers, otherwise known as “polytopic” molecules [1]. Known polytopic molecules are, for instance, the triatomics $\text{M}[\text{CN}]$, metal cyanides ($\text{M}-\text{CN}$) and isocyanides ($\text{M}-\text{NC}$), where M is an alkali or a 3d-transition metal element, the reason being the strong ionic character of such systems.

In the present work we study by post Hartree–Fock methods in conjunction with quantitative basis sets the two isomers Sc–CN (cyanide) and Sc–NC (isocyanide), both experimentally undetected. There exists a recently published computational work by Rayón et al. [2] on the ground states of the $\text{M}[\text{CN}]$ 3d-transition metal series, $\text{M} = \text{Sc} - \text{Zn}$; this is the only study on Sc[CN]. These workers examined the $\text{M}[\text{CN}]$ sequence through density functional theory (DFT/B3LYP), quadratic CI (QCISD), and single point multireference (MRCI) and coupled-cluster (CCSD(T)) calculations using mainly 6-311+G(d) basis sets. They report geometries, harmonic frequencies, dipole moments, and binding energies presenting as well a complete and informative account of previous experimental and theoretical studies of $\text{M}[\text{CN}]$ systems; see also Refs. [3,4].

It is quite interesting that in Sc[CN] and Ti[CN] the most stable isomers are the isocyanides, where in Cr[CN], Co[CN], Ni[CN], and Cu[CN] the energetically lowest are the cyanides. For the V[CN], Mn[CN], and Fe[CN] complexes the two isomers are quasi degenerate the isocyanides lying lower by less than 1 kcal/mol; see Ref. [2] and references cited therein.

The purpose of the present report is a systematic *ab initio* study of the structure and bonding of the ground and low-lying states of ScCN and ScNC isomers.

The Balabanov–Peterson [5] correlation consistent basis set of quadruple cardinality was used for Sc, while for C and N the corresponding augmented quadruple basis sets of Dunning were employed [6], generally contracted to $[\text{}8\text{}s\text{}7\text{}p\text{}5\text{}d\text{}3\text{}f\text{}2\text{}g\text{}1\text{}h\text{}/\text{}_{\text{Sc}}\text{}6\text{}s\text{}5\text{}p\text{}4\text{}d\text{}3\text{}f\text{}2\text{}g\text{}/\text{}_{\text{C,N}}] \equiv \text{}A4\zeta$, a total of 264 spherical Gaussians. The methods used are single reference (restricted Hartree–Fock) valence configuration interaction (RHF + single + double replacements = RHF + 1 + 2 = CISD) and coupled cluster + 1 + 2 + perturbative connected triples = RCCSD(T) [7]. Because of the strong ionic character of both isomers Sc[CN], CISD + Q (+Q = the Davidson correction [8]) and analogous multireference (complete active space self consistent field + 1 + 2 = CASSCF + 1 + 2 = MRCI) calculations, give very similar results around equilibrium. As a matter of fact MRCI calculations along the Sc–[CN] coordinate are plagued by methodological and conceptual problems. No core ($1\text{}s^2/\text{}_{\text{C,N}}$, $1\text{}s^2\text{}2\text{}s^2\text{}2\text{}p^6\text{}3\text{}s^2\text{}3\text{}p^6/\text{}_{\text{Sc}}$), scalar relativistic, and basis set superposition effects have been taken into account judged as unimportant for the purpose of the present work.

We have calculated a total of 20 states, 10 for ScCN and 10 for ScNC. We report energetics, geometries, dipole moments, and harmonic frequencies.

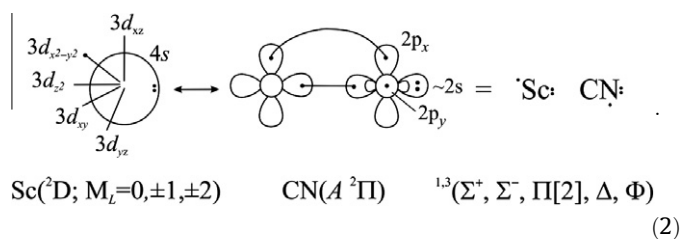
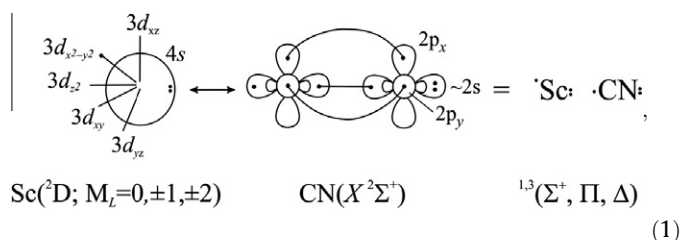
All calculations have been done by the MOLPRO package [9] under $\text{}C_{2v}$ and $\text{}C_1$ symmetry.

2. Chemical insights

The ground states of Sc and CN are ${}^2\text{D}(4\text{}s^2\text{}3\text{}d^1)$ and $\text{}X^2\Sigma^+$ with their first excited states ${}^4\text{F}(4\text{}s^1\text{}3\text{}d^2)$ and $\text{}A^2\Pi$ 1.427¹⁰ and 1.146 eV [11] higher, respectively. The Sc + [CN] (${}^2\text{D} + \text{}X^2\Sigma^+$, ${}^2\text{D} + \text{}A^2\Pi$, ${}^4\text{F} + \text{}X^2\Sigma^+$) interaction along the CN internuclear axis gives rise to ${}^1,3(\Sigma^+, \Pi, \Delta)$, ${}^1,3(\Sigma^+, \Sigma^-, \Pi[2], \Delta, \Phi)$ and ${}^3,5(\Sigma^-, \Pi, \Delta, \Phi)^{2\text{S}+1}\Lambda$ molecular states, respectively from either end of the CN radical. It is expected that the interaction $\text{Sc}(\text{}^2\text{D}) + [\text{CN}](\text{}X^2\Sigma^+, \text{}A^2\Pi)$ to be of repulsive nature as shown by the valence-bond–Lewis (vbL) diagrams (1) and (2).

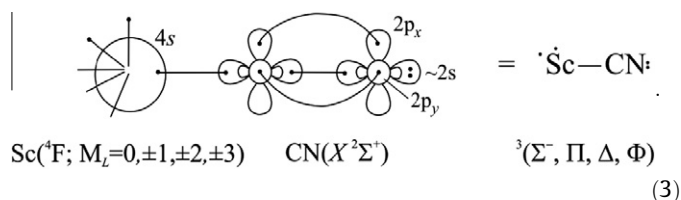
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Notice that the *in situ* C atom in the $X^2\Sigma^+$ and $A^2\Pi$ states of CN finds itself in the 5S and 3P states, respectively. Obviously the approach of CN to $\text{Sc}(^2\text{D})$ from the N-end (isocyanide) leads to repulsive states as well (but see below).

The next channel $\text{Sc}(^4F) + \text{CN}(X^2\Sigma^+)$ from the C-end of the CN group leads to attractive interaction, as it is clearly captured by the vBL icon (3)



The corresponding quintets, that is, $^5(\Sigma^-, \Pi, \Delta, \Phi)$ resulting by coupling the two σ electrons of the Sc-CN “bond” into a triplet, should be repulsive. Finally, the isocyanide attack leads also to repulsive states according to the analogous diagrams (1)–(3).

The bonding analysis above, however, which is based to a prevailing covalent scheme, is undermined by the almost completely ionic Sc^+CN^- “bonding” character around equilibrium, the result of the very high electron affinity (EA) of the CN group combined with the low ionization energy (IE) of Sc, EA = 3.862 eV [12] and IE = 6.562 eV. [10] Thus, it is more natural to consider that the $^{2S+1}\Lambda$ states of $\text{Sc}[\text{CN}]$ result from the $\text{Sc}^+(^3\text{D}, ^1\text{D}, ^3\text{F})$ terms in the field of the “structureless”, negatively charged $\text{CN}^-(X^1\Sigma^+)$ rod; $\Delta E[^1\text{D}(4s^13d^1) \leftarrow ^3\text{D}(4s^13d^1), ^3\text{F}(3d^2) \leftarrow ^3\text{D}] = 0.302, 0.596$ eV. [10] The $\text{Sc}^+(^3\text{D}, ^1\text{D}, ^3\text{F})$ in the field of $[\text{CN}]^-$ gives rise to $^3(\Sigma^+, \Pi, \Delta)$, $^1(\Sigma^+, \Pi, \Delta)$, and $^3(\Sigma^-, \Pi, \Delta, \Phi)$ molecular states, respectively, a total of 10 ScCN and 10 ScNC states. Based on the $\text{Sc}^+[\text{CN}]^-$ model we have studied here all 10 + 10 Sc[CN] states, dissociating adiabatically to $\text{Sc}(^2\text{D}) + [\text{CN}](X^2\Sigma^+)$ ($^1,3\Sigma^+$, $^1,3\Pi$, $^1,3\Delta$) and $\text{Sc}(^2\text{D}) + [\text{CN}](A^2\Pi)$ ($^3\Sigma^-, ^3\Pi$, $^3\Delta$, $^3\Phi$). Therefore the character of these states around equilibrium is due to the interaction of covalent and ionic energy potential surfaces (profiles) of the same symmetry.

We believe that, *mutatis – mutandis*, the previous analysis holds true for the whole $\text{M}[\text{CN}]$ series, $\text{M} = \text{Sc} - \text{Cu}$.

3. Results and discussion

Tables 1 and 2 collect numerical results for the ScCN and ScNC isomers, respectively, whereas Fig. 1 shows the corresponding energy level diagrams. The manifold of the 10 states of ScCN(ScNC) span an energy range of 38.7(41.5) kcal/mol at the CISD + Q level.

$\bar{X}^3\Delta$. According to Tables 1 and 2 the isocyanide is the most stable isomer between the two by 5.8(4.5)[4.4] kcal/mol at the CISD(+Q)[RCCSD(T)] level. Similar results have been obtained by the authors of Ref. [2] concerning the stability of two species as well as with the rest of parameters of the $\bar{X}^3\Delta$ state; see Tables 1

Table 1

Total energies $E_e(E_h)$, geometries $r_e(\text{\AA})$, dissociation energies $D_e(\text{kcal/mol})$, harmonic frequencies $\omega_e(\text{cm}^{-1})$, dipole moments $\mu(\text{Debye})$, and energy separations $T_e(\text{kcal/mol})$ of ScCN at the CISD(+Q)[RCCSD(T)] levels of theory.

State	$-E_e$	$r_e(\text{Sc}-\text{C})$	$r_e(\text{C}-\text{N})$	D_e^a	$\omega_1/\omega_2/\omega_3/\omega_4$	μ^b	T_e
$\bar{X}^3\Delta$	852.475 09	2.288	1.154	96.0	386/2300/154/154	5.9	0.0
	(852.514 47)	(2.284)	(1.164)	(95.0)			(0.0)
	[852.527 88]	[2.282]	[1.170]	[98.3]	[380/2156/133/133]	[6.2]	[0.0]
		2.281 ^c	1.166 ^c	96.42 ^c	379/2165/138/138 ^c		
$^1\Sigma^+$	852.463 92	2.196	1.153	89.0	408/2308/170/170	5.7	7.01
	(852.508 48)	(2.183)	(1.163)	(91.2)			(3.76)
$^2\Sigma^+$	852.468 12	2.274	1.155	91.6	378/2291/170/150	5.9	4.37
	(852.508 03)	(2.266)	(1.165)	(90.9)			(4.04)
	[852.521 83]	[2.261]	[1.171]	[94.5]	[373/2143/160/141]	[6.0]	[3.80]
$^3\Sigma^+$	852.462 42	2.296	1.154	88.1	387/2301/149/149	4.7	7.95
	(852.502 79)	(2.294)	(1.164)	(87.6)			(7.33)
$^4\Sigma^+$	852.454 55	2.269	1.155	83.1	376/2289/151/151	6.2	12.89
	(852.495 98)	(2.260)	(1.165)	(83.4)			(11.60)
$^5\Sigma^+$	852.454 62	2.332	1.154	83.2	353/2290/259/259	5.0	12.85
	(852.494 50)	(2.325)	(1.165)	(82.4)			(12.53)
	[852.508 33]	[2.322]	[1.171]	[86.0]		[4.8]	[12.27]
$^6\Sigma^+$	852.416 45	2.318	1.156	77.0	353/2280/149/149	9.7	36.80
	(852.458 13)	(2.309)	(1.166)	(81.7)			(35.35)
$^7\Sigma^+$	852.414 87	2.304	1.156	76.0	350/2272/149/149	9.3	37.79
	(852.456 89)	(2.292)	(1.166)	(81.0)			(36.13)
$^8\Sigma^+$	852.412 94	2.320	1.156	74.8	350/2280/978i/978i	8.9	39.00
	(852.454 97)	(2.309)	(1.166)	(79.8)			(37.34)
$^9\Sigma^+$	852.410 93	2.332	1.155	73.5	347/2291/836i/836i	8.4	40.26
	(852.452 88)	(2.323)	(1.165)	(78.5)			(38.65)

^a D_e with respect to the adiabatic fragments; see text.

^b μ calculated as expectation value at the CISD level of theory, by the finite field method at the RCCSD(T) level of theory. Field strengths: $10^{-6} - 5 \times 10^{-5}$ a.u.

^c Ref. [2]; the dissociation energy reported corresponds to D_0 .

Table 2
Total energies $E_e(E_h)$, geometries $r_e(\text{\AA})$, dissociation energies $D_e(\text{kcal/mol})$, harmonic frequencies $\omega_e(\text{cm}^{-1})$, dipole moments $\mu(\text{Debye})$, and energy separations $T_e(\text{kcal/mol})$ of ScNC at the CISD(+Q)[RCCSD(T)] levels of theory.

State	$-E_e$	$r_e(\text{Sc-N})$	$r_e(\text{N-C})$	D_e^a	$\omega_1/\omega_2/\omega_3/\omega_4$	μ^b	T_e
$\tilde{X}^3\Delta$	852.484 34 (852.521 67) [852.534 87]	2.125 (2.127) [2.125] 2.123 ^c	1.169 (1.178) [1.183] 1.180 ^c	101.8 (99.5) [102.7] 100.95 ^c	447/2188/98/98 [443/2071/98/98] 437/2086/95/95 ^c	5.3 [5.8]	0.0 (0.0) [0.0]
$1^1\Sigma^+$	852.474 30 (852.517 15)	2.031 (2.026)	1.171 (1.180)	95.5 (96.7)	481/2174/82/82	4.5	6.30 (2.84)
$2^3\Pi$	852.474 19 (852.512 15) [852.525 70]	2.132 (2.130) [2.126]	1.169 (1.178) [1.183]	95.5 (93.5) [96.9]	435/2186/117/140 [426/2060/99/121]	5.4 [5.6]	6.37 (5.97) [5.75]
$3^1\Delta$	852.471 48 (852.509 81)	2.132 (2.134)	1.169 (1.178)	93.8 (92.0)	448/2186/92/92	4.1	8.07 (7.44)
$4^3\Sigma^+$	852.461 11 (852.499 02) [852.512 49]	2.171 (2.170) [2.168]	1.170 (1.179) [1.184]	87.2 (85.3) [88.6]	405/2174/57/57	4.4 [4.3]	14.58 (14.21) [14.04]
$5^1\Pi$	852.459 33 (852.498 74)	2.135 (2.133)	1.168 (1.177)	86.1 (85.1)	428/2189/104/104	5.8	15.69 (14.39)
$6^3\Phi$	852.420 31 (852.460 72)	2.172 (2.168)	1.168 (1.177)	79.4 (83.4)	396/2190/95/95	8.8	40.18 (38.25)
$7^3\Sigma^-$	852.416 65 (852.457 38)	2.182 (2.175)	1.167 (1.177)	77.1 (81.3)	394/2192/82/82	8.5	42.48 (40.34)
$8^3\Pi$	852.415 74 (852.456 44)	2.182 (2.176)	1.168 (1.177)	76.5 (80.7)	392/2190/528i/ 528i	8.3	43.05 (40.93)
$9^3\Delta$	852.414 99 (852.455 47)	2.179 (2.176)	1.168 (1.177)	76.1 (80.1)	391/2191/1145i/1145i	7.9	43.52 (41.54)

^a D_e with respect to the adiabatic fragments; see text.

^b μ calculated as expectation value at the CISD level of theory, by the finite field method at the RCCSD(T) level of theory. Field strengths: $10^{-6} - 5 \times 10^{-5}$ a.u.

^c Ref. [2]; the dissociation energy reported corresponds to D_0 .

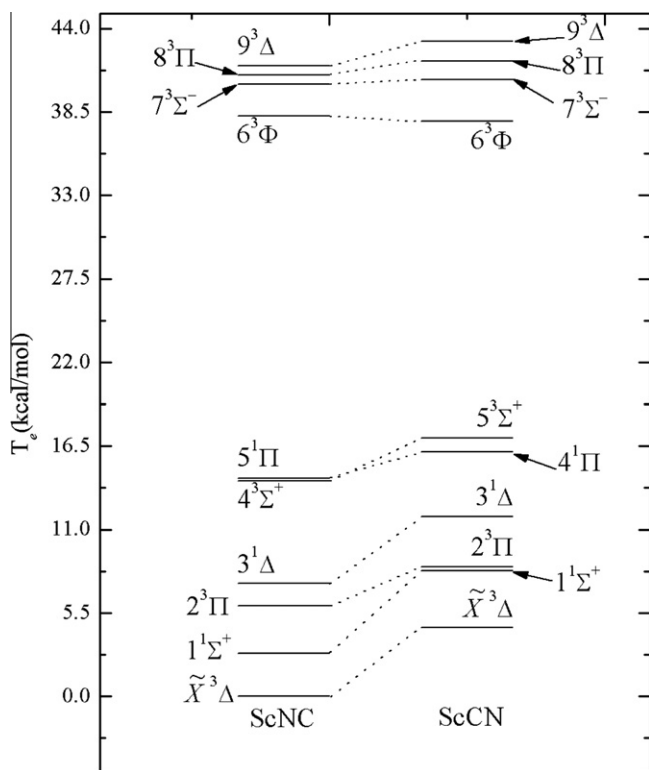


Fig. 1. Relative energy level diagram of ScNC and ScCN at the CISD + Q/AQ level.

and 2. The leading CISD equilibrium configuration for both isomers and corresponding Mulliken populations are (only valence electrons are counted)

$$|\tilde{X}^3\Delta\rangle \approx 0.95 |1\sigma^2 2\sigma^2 3\sigma^2 4\sigma^1 1\pi_x^2 1\pi_y^2 1\delta^1\rangle \\ \approx \hat{A}\Psi(\text{Sc}^+; ^3\text{D}) \times \Psi(\text{CN}^-; X^1\Sigma^+),$$

$$\text{ScCN} : 4s^{0.91} 4p_z^{0.35} 3d_{z^2}^{0.16} 3d_{xy}^{1.0} /_{\text{Sc}} 2s^{1.20} 2p_z^{1.05} 2p_x^{0.82} 2p_y^{0.82} \\ /_{\text{C}} 2s^{1.89} 2p_z^{1.36} 2p_x^{1.11} 2p_y^{1.11} /_{\text{N}},$$

$$\text{ScNC} : 4s^{0.84} 4p_z^{0.25} 3d_{z^2}^{0.11} 3d_{xy}^{1.0} /_{\text{Sc}} 2s^{1.64} 2p_z^{1.06} 2p_x^{0.55} 2p_y^{0.55} \\ /_{\text{C}} 2s^{1.78} 2p_z^{1.25} 2p_x^{1.36} 2p_y^{1.36} /_{\text{N}}.$$

A total of 0.60 (Sc—C—N) and 0.75 (Sc—N—C) electrons are transferred from the metal to the CN group, the charge on the C atom being practically zero. Within ~ 0.01 Å the bond distance of the *in situ* CN group is the same in both isomers, very similar to the bond distance of the free $\text{CN}^-(X^1\Sigma^+)$ anion, 1.173(1.179) Å at the CISD+Q(RCCSD(T)) level. The experimental bond length of $\text{CN}^-(X^1\Sigma^+)$ is 1.177 Å. [11] The considerably smaller distance of Sc—NC as compared to Sc—CN by 0.16 Å (see Tables 1 and 2), and the localization of the negative charge on the N atom, is perhaps, the cause of the increased stability of the former with respect to the latter by ~ 5 kcal/mol (*vide supra*). Although the bonding is mainly ionic in nature for both isomers, a $(4s4p_z 3d_{z^2})^{1.4}$ hybrid (ScCN) vs $(4s4p_z 3d_{z^2})^{1.2}$ (ScNC), suggest a weak covalent interaction as well in the cyanide case.

Higher states. For both isomers the 10 Sc[CN] states are naturally divided into two groups of 6 + 4 states within energy ranges of 14.4 and 3.3 (ScNC), and 12.5 and 3.3 (ScCN) kcal/mol, respectively at the CISD+Q level; see Tables 1 and 2 and Fig. 1. The first 6 states of Sc[CN] correlate adiabatically [diabatically] to $\text{Sc}(^2\text{D}; 4s^2 3d^1) + \text{CN}(X^2\Sigma^+)$ [$\text{Sc}(^3\text{D}, ^1\text{D}) + \text{CN}(X^1\Sigma^+)$], while the cluster of the 4 upper states to $\text{Sc}(^2\text{D}) + \text{CN}(A^2\Pi)$ [$\text{Sc}(^3\text{F}) + \text{CN}(X^1\Sigma^+)$].

For all 10 states of ScCN and ScNC the CISD+Q CN bond length is practically invariant to the molecular symmetry, being 1.165 and

1.178 Å, respectively. This distinct difference of ~ 0.015 Å in the CN bond length among the cyanides and isocyanides, is rather due to the higher ionic character of the iso-isomer; recall that the $\text{CN}^-(X^1\Sigma^+)$ CISD+Q bond length is 1.173 Å. This CISD+Q difference of ~ 0.015 Å is maintained as well at the RCCSD(T) level of theory, at least for the three states studied at this level ($\tilde{X}^3\Delta$, $^3\Pi$, $^3\Sigma^+$). As to the Sc–CN and Sc–NC bond length differences, with the exception of the $^1\Sigma^+$ Sc[CN] state, the former is longer than the latter by ~ 0.15 Å perhaps due to the more pronounced Coulombic interaction in the ScNC isomer. The average Mulliken charge, practically the same in all 20 Sc[CN] states, is $\overset{+0.5}{\text{Sc}} - \overset{0.0}{\text{C}} - \overset{-0.5}{\text{N}}$ and $\overset{+0.75}{\text{Sc}} - \overset{-0.70}{\text{N}} - \overset{-0.05}{\text{C}}$.

Our recommended D_e values for the \tilde{X} states are those obtained at the coupled-cluster level, 98 (ScCN) and 103 (ScNC) kcal/mol. Corresponding D_0 values are $D_0 = D_e - \sum_{i=1}^4 \omega_i/2$ (Sc[CN]) + $\omega_e/2$ (CN) = 97.3 and 101.8, respectively. A comment is in order at this point concerning the dipole moments. First, the dipole moments of ScCN are on the average larger than the ones of ScNC by 0.5–1.0 Debye, perhaps due to the larger distance of the localized charges on the Sc and N atoms. Second, observe that the dipole moments of the 4 upper states for both isomers are approximately twice as large as those of the 6 lowest states.

Finally the four harmonic frequencies ω_1 , ω_2 , ω_3 , and ω_4 listed in Tables 1 and 2, mirror the Sc–[CN] and the Sc[C–N] stretchings, and the two perpendicular bending modes, respectively. Observe that the two bending modes are practically degenerate reflecting the ionic character of the Sc[CN] system.

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