

Re: Oxidation number of atoms in thiocyanate ion

Source: <http://sci.tech-archive.net/Archive/sci.chem/2004-10/1127.html>

farooq_w_at_hotmail.com

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photo@woelen.nl wrote:

> farooq_w@hotmail.com wrote:

> > photo@woelen.nl wrote:

> >

> > > This is new to me. I thought that oxygen bonding was limited to

> > double

> > > bonds. Is this third bond a real bond?

> > triple bond = one sigma bond + two pi bonds.

> I'll look up what this means for the distribution of electrons. My

> knowledge of the different bonding types is buried deeply, although

> once, I grasped the idea behind it.

> >

> > > > For molecules like NO and NO2 I have the same problem when

> making

> > > Lewis

> > > > dot-structures,

> >

> > NO is said to have a bond order of 2.5(two double bonds + one odd

> > electron)

> >

>

>

>

>

> >

> > Can you do me a favor if you spare few minutes to solve this
problem

> > with a computer program to 8 decimal places, if it not so cubersome

> for

> > you. I just need to check, because neither I nor the the teacher
have

> > been able to get the correct answer perhaps the large number of
> decimal

> > places are required and rounding off gives a significant error.

> >

> > The system is:

> > [Ca] 146.12 + [Ba] 193.66 + [Sr] 243.36 = 0.56246

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> > [Ca] 128.10 + [Ba] 175.64 + [Sr] 225.35 = 0.50980
> > [Ca] 100.09 + [Ba] 147.63 + [Sr] 197.34 = 0.42730
>
> *The set of equations, you supplied is singular within the given
> accuracy:*
> *The singular value decomposition (SVD) of the matrix on the left hand
> is*
> 5.3546e+02
> 1.2642e+01
> 1.9671e-03
> *The largest eigenvalue of sqrt(AA') is more than 10⁵ times as large
as*
> *the smallest one. This means that you loose approximately 5 digits of
> significance, when determining the numerical solution of this system.*
> *Because you only have 5 digits, one can safely state that this system
> is singular within the given precision. The SVD shows that you have
two*
> *independent relations, the third one is just a combination of the
other*
> 2.
>
> *For your information:*
> *The third equation can be written as eq3 = eq2 - a*(eq1 - eq2) within
> the given accuracy of 5 digits, where a = 1.554384.*
> *E.g. 100.09 = 128.10 - a*(146.12 - 128.10). The same relation exists
for*
> *all other coefficients.*
>
>
> *Nevertheless, I can supply you with a solution, computed at 15 digit
> accuracy internally, but I'm afraid this solution is meaningless:*
> [Ca] = 0.04362447
> [Ba] = -0.08224782
> [Sr] = 0.04156873
>
> *I'm wondering, don't you have computer hardware and software, with
> which you can solve this type of problems? There are quite some good
> open source products out there, such as Octave, pari/gp and libraries
> like GSL.*

Thank you Wilco. I will show this solution to him (he said the he never got the correct answer...perhaps he didn't think of eq3 = eq2 - a*(eq1 - eq2). This was a problem of a mixture of calcicum , barium and strontium oxalates where were heated and the weight loss was recorded at three different temperatures and hence three equations. This is called thermogravimetric analysis.

Wilco, you would be surprised (but shouldn't be for someone from Pakistan) that I am hearing of those names for the first time. I lag behind atleast 20 years :-(.