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   KRA - substitution coordinates from single isotopic substitution in
         a linear/symmetric/asymmetric top from Kraitchman's equations

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       - The program uses single isotopic equations straight out of
         Gordy&Cook
       - Experimental errors in rotational constants are propagated into
         errors in coordinates
       - The much more realistic errors according to the Costain criterion
         are then added to the errors above,
       - For planar molecules suitable planarity conditions can be built in
         to use any two out of the three measured constants

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    Input:

    MOLNAM.KRA - The input file with name specified in response to the prompt
                 from the program. The use of the extension .KRA is recommended.

    Output:

    MOLNAM_KRA.OUT - main output file

    MOLNAM_KRA.EVA - stub file for the EVAL program containing the coordinates
                     and their uncertainties evaluated by KRA.
                     It is still necessary to assign signs, add two preceding
                     lines containing the descriptive comment and the number
                     of atoms, and append lines with declarations of internals
                     that are to be evaluated
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    The syntax of the input file:

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    line0:     comment line
    line1:     i   j
    line1a:    k   l
    line2:     A,  dA     \
    line2a:    B,  dB      |- for the parent species
    line2b:    C,  dC      |
    line3:     Mass       /
    line4:     A,  dA     \
    line4a:    B,  dB      |- for a substituted species
    line4b:    C,  dC      |
    line5:     dMass      /
        .
        .
    lastline:  end
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   - Line1 selects the type of top:

     i=0: defines that the parent is a diatomic, linear or a symmetric top
          (off-axis asymmetric substitution is allowed for a symmetric top)

If i=0 then the value of j is irrelevant but is still necessary on
input so it is best to also set it to zero.

i>0: defines that the parent is an asymmetric top, in which case i and j
i<0 can take values out of 1,2,3 (i.e. a,b,c). i cannot be equal to j,
and (i,j) selects the inertial plane for planar coordinate
calculation.
One of i and j can be negative in which case the respective moment
of inertia is calculated using the planar relation defined in line1a

- Line1a is only necessary if one of i,j is negative and defines the
planar relation for calculation of that moment. For the most common case
of a planar molecule in the ab inertial plane there are three alternatives:

line1 i,j:	1 2	-1 2	1 -2
line1a k,l:	none	3 -2	3 -1

and, for example, k,l = 3 -2 define I.a = I.c - I.b
For a non-zero inertia defect each these three cases gives a slightly
different result in the 'PLANAR' section, while the results in
the 'NONPLANAR' section will be identical.

- Line 2: rotational constant A and its error dA for the parent species (MHz).
If the species is not an asymmetric top then set A to a value
large enough to pretend that it is infinity, say to 9999999.0

- Line 2a: B, dB for the parent (MHz)
- Line 2b: C, dC for the parent (MHz)

- Line 3: mass of the parent isotopic species in u

- Lines 4: rotational constant A and its error dA for the substituted
species (MHz)

- Line 4a: B, dB for the substituted species (MHz)
- Line 4b: C, dC for the substituted species (MHz)

- Line 5: the mass difference between the mass of substituted species and
that of the parent species (u), see the table below for some
common values.

- Lines 4-5 can be repeated as many times as necessary, and are best
terminated with a line beginning with the word 'end'
(without the inverted commas)

NOTE:

- Lines that begin with a recognised comment flag i.e.
with either one of c,C,#,!,% are ignored so that
comment lines can be inserted anywhere in the data file.
The first line is the only exception as it is always treated as
comment describing the whole data set.

- The X,Y,Z coordinates in the output are consistent with the
x,y,z indices in the equations in Gordy&Cook

- The program tries to extract a six character descriptor from the comment lines
preceding each isotopic species. This descriptor will begin with the first
non blank character after the character defining the comment line.
The descriptor will be carried over to the .EVA file.

- Remember that all substitution coordinates determined with Kraitchman's
equations arise from a square root operation so that their sign is
indeterminate. For convenience KRA prints all coordinates positive, and

not with +- sign in front of each.
It is, of course, necessary to assign signs to coordinates for their
use in determination of internal structural parameters, as for example
with EVAL.

References:

[1] W.Gordy and R.L.Cook, "Microwave Molecular Spectra", Wiley,
New York, 1984.
The relevant substitution relations are:
linear: Eq.13.46
off axis symm.: Eq.13.56-13.57
planar asymm: Eq.13.64-13.65
general asymm. Eq.13.71-13.73
Costain rule Eq.13.183

[2] C.C.Costain, "Further comments on the accuracy of r_s substitution structures",
Trans.Am.Crystallogr.Assoc. 2,157-164(1966).

NOTE: what became the 'Costain rule' started off in the Costain paper
as an estimate of 0.0012/r based on NNO data (p.159).
The generalisation to the form 0.0015/a as found in Gordy&Cook
was made later. A preceding version of the G&C text can be found,
for example, in:

[3] M.D.Harmony, V.W.Laurie, R.L.Kuczkowski, R.H.Schwendeman,
D.A.Ramsay, F.J.Lovas, W.J.Lafferty, A.G.Maki,
"Molecular Structures of Gas-Phase Polyatomic Molecules
Determined by Spectroscopic Methods", J. Phys. Chemn. Ref. Data,
8, 619-721 (1979), p.624.
PDF version (bitmap scan) of that paper is freely available from
the NIST Standard Reference Data under the direct link:
http://www.nist.gov/data/PDFfiles/jpcrd146.pdf

Mass differences for use in KRA:

Updated from "Atomic Weights and Isotopic Compositions" at:
http://www.nist.gov/pml/data/comp.cfm based on primary sources up to 2007

M.parent (u)	M.isot (u)	Delta.M (u)
1.H = 1.00782503207	2.H = 2.0141017778	1.0062767
	3.H = 3.0160492777	2.0082242
12.C = 12.	13.C = 13.0033548378	1.0033548
14.N = 14.0030740048	15.N = 15.0001088982	0.9970349
16.O = 15.99491461956	17.O = 16.99913170	1.0042171
	18.O = 17.9991610	2.0042464
20.Ne = 19.9924401754	21.Ne = 20.99384668	1.0014065
	22.Ne = 21.991385114	1.9989449
28.Si = 27.9769265325	29.Si = 28.976494700	0.9995682
	30.Si = 29.97377017	1.9968436
32.S = 31.97207100	33.S = 32.97145876	0.9993878
	34.S = 33.96786690	1.9957959
	36.S = 35.96708076	3.9950098
35.Cl = 34.96885268	37.Cl = 36.96590259	1.9970499
40.Ar = 39.9623831225	36.Ar = 35.967545106	-3.9948380

	38.Ar = 37.9627324	-1.9996507
79.Br = 78.9183371	81.Br = 80.9162906	1.9979535