Example of non-standard route and input file for Gaussian 98

The following example shows the calculation of molecular properties (NBO analysis and GIAO shielding tensors) with a wave function modified by deletions of specific elements of the Fock matrix in the NBO basis. In the Gaussian 98 calculation, this requires a non-standard route consisting of a sequence of overlays that include:

Line 1: Options related with the specification of nuclear centers.

Line 2: Symmetry specification. It is set to "NoSymmetry", to prevent the molecule reorientation and cause all computations to be performed in the Z-matrix orientation.

Line 3: Basis set information and options related with one- and two-electron integrals required for an SCF calculation.

Line 4: Initial guess to the solution of SCF equations.

Line 5: General information related to the SCF procedure.

Lines 6-7: Request a full NBO analysis (line 6), and a NBO deletion analysis (line 7).

Line 8: Indication for one step of the SCF procedure. This overlay assures the NBO links (link 607, line 7) pass to the ESS (electronic structure system) the density matrix modified by deletions. In this way all subsequent overlays included in the job will be calculated with the density matrix modified by deletions (plus one step of the SCF cycle). Up to this point the route is very similar to a standard route corresponding to a NBO energetic analysis.

Lines 9-12: Calculation of molecular properties, in this case, a NBO localization with default options (line 9), evaluation of the deletion energy (line 10), and the calculation of GIAO magnetic properties. These lines imply an unusual combination of options within a Gaussian job, as all the properties are evaluated with a modified wave function.

An example of a complete input file and sequence of overlays used in the calculations is shown below:

```
#p NonStd
 1/38=1/1;
 2/15=1/2;
 3/5=1,6=6,7=111,11=9,25=1,30=1/1,2,3;
 4/7=1/1;
 5/5=2,32=2,38=4/2;
 6/7=2,8=2,9=2,10=2,19=1,28=1,40=11/1,7;
 6/7=2,8=2,9=2,10=2,19=1,28=1,40=2/7;
 5/5=2,7=1,13=1,38=4/2;
 6/7=2,8=2,9=2,10=2,28=1,40=3/7;
 6/7=2,8=2,9=2,10=2,28=1,40=1/1,7;
 8/6=1,11=11/1;
 10/13=100,33=1/2;
 99/5=1/99;

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Uracil (NBO & NMR) Del5

0  1
N     0.000351    1.172700    1.972305
C     0.000000    0.000000    1.216736
N    -0.000351   -1.142227    2.000977
C    -0.000381   -1.237976    3.411057
C     0.000031    0.059814    4.079285
C     0.000397    1.194809    3.348297
O     0.000000    0.000000    0.000000
O    -0.000717   -2.329346    3.955400
H     0.000641    2.027069    1.432510
H    -0.000565   -2.019928    1.493103
H     0.000061    0.075256    5.160690
H     0.000671    2.183334    3.794876

 $NBO BNDIDX $END
 $DEL DELETE 1 ELEMENT 24 170 $END
```

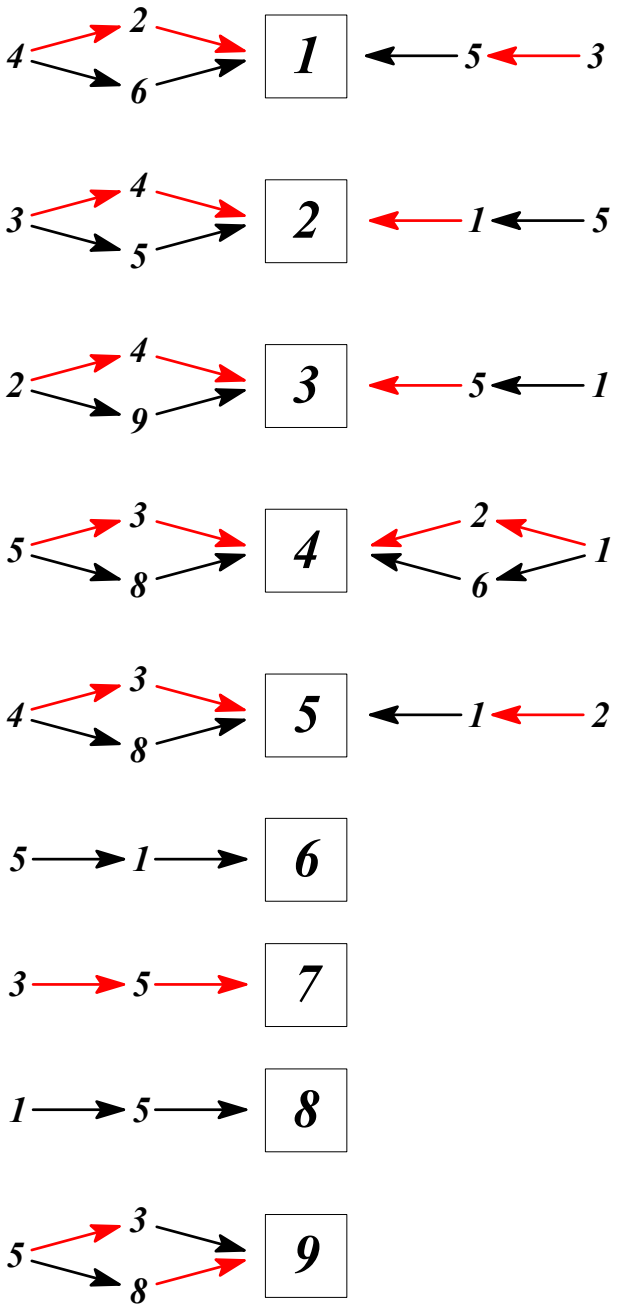

Figure S1. Schematic representations for the main paths of indirect influences on interactions *1*-*9* in uracil (shown in the boxes), for which $\langle \Delta E^{(2)} \rangle$ is greater than 25% of the most intense influence (Figure 5). Each interaction is connected to the next one by a direct influence, black arrows indicate a cooperative influence and red arrows represent an anticooperative influence. Note that in several cases more than one pathway may connect the same initial and final interactions, only the shortest pathways involving significant direct influences are shown. See Figure 2 for notation.

Table S1. Effect of selected stereoelectronic interactions over carbon and oxygen NAOs of uracil carbonyl C_4=O

Atom	**Interaction**	**Δ(*Occupancy*) of valence NAOs**			
		2s	**2p$_x$**	**2p$_y$**	**2p$_z$**
C_4	*1*	–0.0102	0.0220	–0.0086	0.0003
	2	–0.0085	0.0288	–0.0135	0.0030
	6	–0.0037	–0.0253	0.0045	–0.0100
	7	–0.0060	–0.0137	0.0031	–0.0071
O_4	*1*	–0.0033	0.0244	–0.0043	–0.0003
	2	–0.0034	0.0330	–0.0078	–0.0045
	6	–0.0013	0.0365	–0.0290	0.0175
	7	–0.0007	0.0194	–0.0141	0.0099