Accessory Publication

Highly Twisted C=C Double Bonds in 4-Methyleneisoxazolones

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Contents:

1. Rotational barriers abut the exocyclic double bonds C4=C6 in isoxazolones determined by dynamic ^{1}H NMR analysis.

NMR line shape analysis was performed according to Sandström.[1] The ^{1}H NMR spectra of isoxazolone **13** and **20-21** were recorded in DMSO-d_6 at 500 MHz at different temperature intervals, starting at 20°C and increasing the temperature by 5°C increments. The chemical shifts of the methyl protons belonging to the isopropyl groups broadened upon warming. They were monitored until the two peaks merged into a sharp singlet (fast exchange). The intensities of the methine protons were too low to permit reliable measurements. The populations of the exchanging isopropyl groups p_A and p_B are equal, $p_A = p_B = 0.5$. Hence the rate of exchange for the forward and reverse processes are the same, $k_1 = k_{-1}$. As a result, the intensity of the line shape is given by equation (1),[1,2]

$$v = -C_0 \frac{\{P[1 + \tau(\pi\omega)] + Q.R\}}{P^2 + R^2} \qquad (1)$$

where,

$$\Delta v = 0.5(v_A - v_B) - v$$
$$P = \tau[(\pi\omega)^2 - 4\pi^2\Delta v^2 + \pi^2(\delta v)^2] + (\pi\omega)$$
$$Q = \tau[2\pi\Delta v]$$
$$R = 2\pi\Delta v[1 + \tau(2\pi\omega)]$$
$$\delta v = (v_A - v_B)$$

v_A, v_B = chemical shifts (in Hz) of nuclei A and B in the absence of exchange

v = variable frequency (in Hz)

τ = $1/(2k)$ = exchange lifetime (in sec)

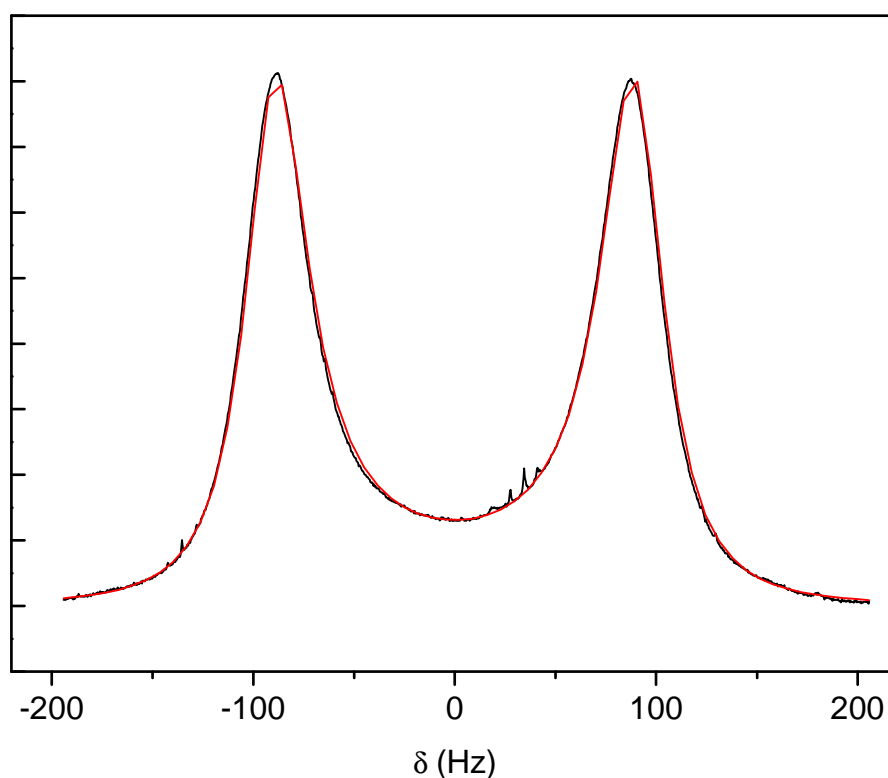ω = width of the signal at half-height (in Hz)

Figure S1. Experimental and simulated (superimposed) NMR spectrum of **13** at 303 K.

In this approach, a non-linear regression analysis was performed using the Levenberg-Marquardt optimisation algorithm which was part of a statistical software.[3] To this aim, equation (1) above was entered into the algorithm of the program, which was used to plot a simulated spectrum. The experimental data was tabulated into frequency-intensity pairs, centered at 0 Hz. The relative intensities are proportional to a scaling factor ($-C_0$), which does not affect the rate. Initial values and boundaries were required for the other variables. Convergence was achieved after a few iterative cycles, given good initial values. Estimates for the half-width (ω) and chemical shift difference (δv) were read directly from the spectra outside of the coalescence range. Approximate rate constants were obtained from the peak separation or ratio methods.[4] The simulated spectra could be fitted very closely to the experimental data ($R^2 \geq 99.5\%$). A typical fit by this method is shown in Figure S1.

The value of k was temperature dependent. As k increased, the shape of the methyl signals broadened and merged into a single, wide, flat-topped resonance, indicating coalescence (Fig. S2). At that temperature, the rate constant is equal to $k_c = [\pi(\delta v)/\sqrt{2}]$, where δv is the chemical shift difference in the absence of exchange (e.g. 180 Hz for **13**) .
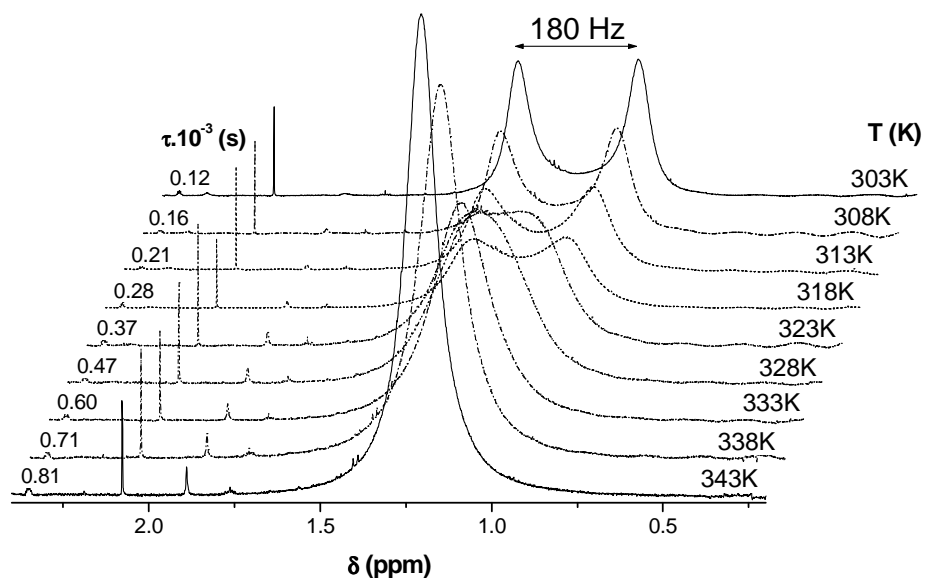
Figure S2. Exchange lifetime τ (sec) as a function of temperature (K) for **13**.

From transition-state theory,[4] it follows that,

$$R.\ln\left(\frac{hk}{k_B T}\right) = \Delta S^{\ddagger} - \Delta H^{\ddagger}\left(\frac{1}{T}\right) \qquad (2)$$

thus the Eyring plot of $R\ln(hk/k_B T)$ versus $(-1/T)$ yields $\Delta S^{\ddagger}$ as the intercept and $\Delta H^{\ddagger}$ as the slope, by least-squares linear regression analysis, (Figure S3).
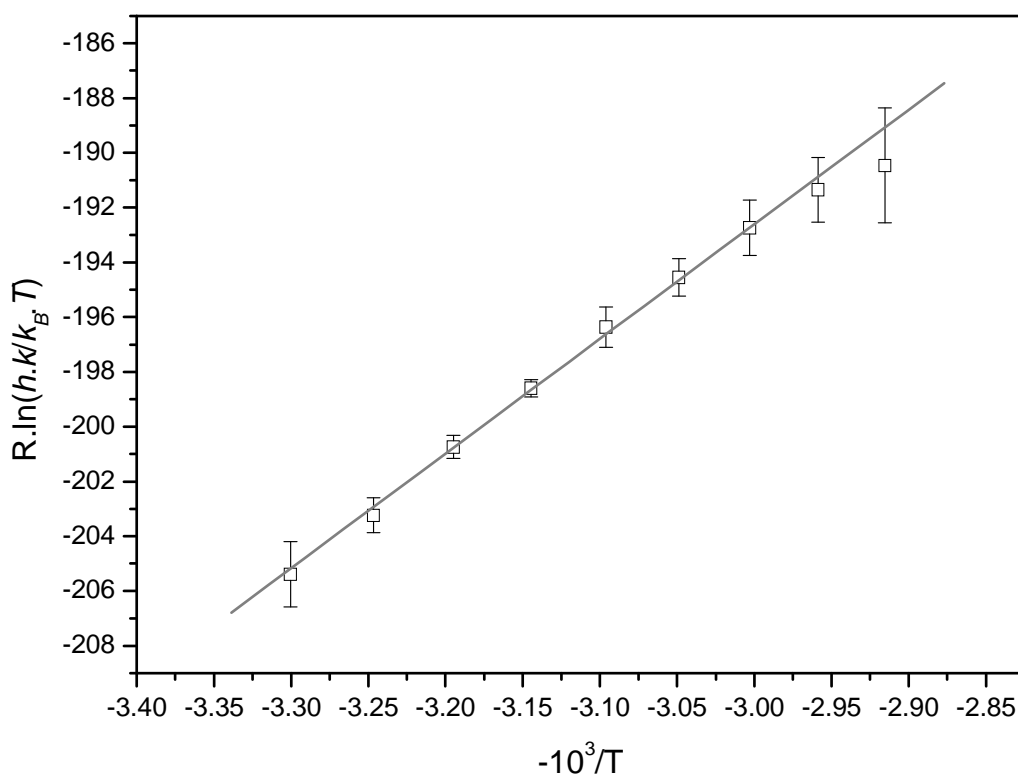
Figure S3. Eyring Plot of Rln (hk/k_BT) versus (-10³/T) for **13** with 95% confidence limits.

The coalescence temperature T_c was calculated from equation (2) and from the activation parameters derived from the Eyring plot. Since T appears in both sides of the equation, an average value from the graph was used. Equation (2) was then iteratively solved for T until the values converged to T_c (e.g. 325 K for **13**). The free energy barrier at the coalescence temperature was then calculated from equation (3),

$$\Delta G^{\ddagger}_{c} = \Delta H^{\ddagger} - T_c \, \Delta S^{\ddagger} \qquad\qquad (3)$$

Since k and T are covariant, the standard deviation in Rln(hk/k_BT) was given by a propagation of errors according to equation (4),

$$\Delta\left(R\ln\left(\frac{hk}{k_B T} \right) \right) = R \sqrt{ \left[\frac{\sigma_k}{k}\left(\ln\left(\frac{hk}{k_B T} \right) + 1 \right) \right]^2 + \left(\frac{\sigma_T}{T} \right)^2 } \qquad (4)$$

The 95% confidence limits[5] in Figure S3 were derived from equation (4) using the standard deviations in the rate constant (σ_k) obtained from the non-linear regression analysis. It can be seen that errors in k are much higher at the extremes of the temperature range than near the coalescence.

The total shape analysis, as opposed to approximate methods, is known to give reliable thermochemical activation parameters.[1] The final data is summarised in Table 3 in the printed paper (**13** and **20-21**: $\Delta H^{\ddagger} =$ 9-10 kcal/mol, $\Delta S^{\ddagger} =$ 16-21 cal K^{-1} mol^{-1}, and $\Delta G^{\ddagger} =$ 15-16 kcal/mol). A related push-pull alkene, 3,3-bismethylthio-2-nitro-acrylonitrile, had a somewhat higher $\Delta H^{\ddagger} =$ 13.1 kcal/mol.[6] Ordinary ketene mercaptals normally have relatively high free energy barriers of rotation, with $\Delta G^{\ddagger}$ in the order of 18-20 kcal/mol and higher.[7] The lower barriers observed here can be ascribed to the superior ability of the isoxazolone ring to stabilize a negative charge in the transition state. Moreover, steric factors may help destabilizing the planar conformation (see structures in the printed paper). The negative entropies of activation are consistent with the highly dipolar nature of the transition state, as a result of the *electrostriction* or dipole-dipole binding of solvent molecules (particularly DMSO, owing to its high dielectric constant). The lower barrier to C=C rotation in **20** compared to **13** is consistent with the cyanophenyl group being able to better stabilise the developing negative charge by increased delocalisation, whereas the lack of an aromatic substituent in **21** may account for the relatively higher free energy of activation; however, the compensating natures of $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ (Table 3) render further analysis of small effects unwarranted.

1.   Sandström, J., *Dynamic NMR Spectroscopy*. Academic Press: London, **1982**.
2.   Rogers, M. T.; Woodbrey, J. C. *J. Phys. Chem.* **1962,** *66*, 540.
3.   *Origin*, 6.0; Microcal Software, Inc: Northampton, MA, USA, **1991-1999**.
4.   Laidler, K. J.; Meiser, J. H., *Physical Chemistry*. 3rd ed.; Houghton Mifflin Company: Boston, **1999**.
5.   Skoog, D. A.; West, D. M.; Holler, F. J., *Fundamentals of Analytical Chemistry*. 7th ed.; Saunders College Publishing: Orlando, **1996**.
6.   Dreier, C.; Henriksen, L.; Karlsson, S.; Sandström, J. *Acta Chem. Scand.* **1978,** *B 32*, 281.
7.   Sandström, J. *Top. Stereochem.* **1983**, *14*, 83.

2. Computational details

The following entries consist of the label, according to the main manuscript, the total energy in Hartrees and the Cartesian coordinates of the optimised structure. A label of **x_SCRF** refers to a structure optimised in a solvent field; **x_rot_ts** refers to the rotational transition states calculated to derive activation barriers (imaginary frequencies (cm^{-1}) given in parenthesis).
Details of the NBO population analysis are given in Table S1 and Figure S4.

12:
E_{tot}=-1465.4159509

N 0.876155254 2.6101361059 -0.4878253868
C 0.6770685516 1.3554861656 -0.1865369581
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C 4.0066123103 -0.1680101523 -1.1121561842
C 2.8433876227 0.5981201066 -1.1626541713
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C 3.2260439104 -1.1389405131 1.0094177877
C -0.7197374367 1.1211530545 0.1710802594

C 4.1784831683 -1.0729934672 -0.0111087849
C -1.4306468596 -0.0361848782 0.4628850359
C 3.9742783201 -0.2210087299 -1.1001434998
C 2.818952204 0.5570961113 -1.1728034642
C -1.3294795936 2.4537888856 0.1326349403
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C -0.2531618738 -1.4671633802 -1.6957535146
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C -2.9071051412 -2.0003550538 -0.0357805409
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13_rot_ts:
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14:
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O -0.7894351944 3.1206853962 -0.2106881049
C 1.6533400454 0.4873628485 0.0537968018
C 1.8017620461 -0.467213555 1.0721831704
C 2.9950374163 -1.1766954995 1.2022909426
C -0.9701044273 0.8755303237 0.0284790368
C 4.0524247254 -0.9420006326 0.3180575146
C -1.5600675921 -0.4015512206 -0.0181704037
C 3.9132236739 0.011907677 -0.6929775157
C 2.720951137 0.7253293694 -0.8240479908
C -1.7252636496 2.1113967368 -0.0682204113
O -2.9208319071 2.3700891888 -0.113625063
N -2.7110402844 -0.6908311255 0.5948121787
S -0.7791270957 -1.6399006592 -1.0064383295
C -1.1292242245 -3.2097700768 -0.1242007166
C -3.2934074228 0.0730525865 1.6998927488
H 0.9905646135 -0.6407497408 1.7757611323
H 3.1012350551 -1.9112317912 1.9989194668
H 4.9821747093 -1.4996810389 0.4190999666
H 4.733038939 0.200307972 -1.3843244
H 2.6073833414 1.4641761249 -1.6140136043
H -3.2591584139 -1.4799937955 0.2521473682
H -2.1639661701 -3.5366009381 -0.2508928676
H -0.881984629 -3.113160366 0.935281359
H -0.4675170174 -3.9481930468 -0.5846975724
H -3.908194119 0.8971418644 1.3309677071
H -2.4855278981 0.4854863114 2.3097304064

H -3.8920915088 -0.6139682508 2.3025150425

14_rot_ts:
E_{tot}=-1122.5589548 (-123.2 cm^{-1})

N -0.4331927311 -2.4078636487 0.1875337538
C -0.2445177283 -1.2407767153 0.7634101301
O 0.7333615509 -2.7120681946 -0.526251172
C -1.3350102117 -0.6571011087 1.5715458417
C -1.1241897938 0.4172801576 2.4477419063
C -2.1736062772 0.9452669701 3.2013941678
C 1.0584239623 -0.7247220011 0.4678123931
C -3.4543714473 0.4047932507 3.0947289974
C 1.7069323769 0.5179661315 0.7549259879
C -3.6762116614 -0.6688372545 2.2269497152
C -2.6318893334 -1.192852132 1.4718062446
C 1.6835765931 -1.6950671825 -0.3990760084
O 2.7742914058 -1.7503711952 -0.9409280296
N 2.5013002465 0.7081037012 1.7988029809
S 1.4723617797 1.7592938398 -0.4363616233
C 2.5234707104 3.1772683074 0.0791876598
C 2.8192214703 -0.3022076833 2.8104624051
H -0.1319545824 0.8450060838 2.5556478381
H -1.9869351919 1.7781094036 3.8748053024
H -4.2728003234 0.815461624 3.6799152274
H -4.6711730028 -1.0964051587 2.1345408719
H -2.7985700255 -2.0220754357 0.7929047465
H 2.9583377618 1.6075147451 1.9081743928
H 3.58053242 2.8959564944 0.106546763
H 2.2006735546 3.5928487848 1.0388789172
H 2.3904602542 3.9429838341 -0.6892928713
H 3.9048068032 -0.4184833021 2.8721490439
H 2.3607126713 -1.2423333753 2.5068589042
H 2.4263884495 0.0084989097 3.7835971537

15:
E_{tot}= -858.3759581

N 0.4802426322 2.7374999817 -0.7967587639
C 0.3612853818 1.4919967425 -0.4137593848
O -0.8162619037 3.2089766881 -1.1021638829
C 1.5793272605 0.7772139102 0.0244216559
C 1.5491792163 -0.1227918807 1.1014533185
C 2.7128761501 -0.7695581938 1.517864086
C -1.0168299677 1.062557386 -0.4005498759
C 3.9242353134 -0.523261018 0.8683651496
C -1.5986755078 -0.2014268105 -0.209852447
C 3.9656317591 0.380039189 -0.1964325888
C 2.8039514473 1.0249046141 -0.6166066739
C -1.7656724441 2.2284860738 -0.8464536212

O -2.9501969835 2.4272938735 -1.0531086872
N -2.833692245 -0.328412881 0.356763416
N -0.9778660357 -1.3627945567 -0.59565642
C -1.0814006112 -2.5978927002 0.1716964371
C -3.8177415319 -1.2871036384 -0.1404476604
C -3.3704219292 0.6729144163 1.2755383203
C -0.0811059726 -1.4262039882 -1.744276491
H 0.6160196276 -0.296111986 1.6292400893
H 2.6756255233 -1.4568925207 2.3591965203
H 4.8302944096 -1.0278338619 1.1930041378
H 4.9056135642 0.5813763221 -0.703335637
H 2.8283873463 1.7291557742 -1.4419237583
H -1.6022521117 -3.387021324 -0.3870439931
H -1.6171528299 -2.4119887823 1.1032220442
H -0.0727208852 -2.9576885542 0.4124969149
H -4.1114711513 -2.0058333874 0.635276022
H -3.4146240687 -1.8288311966 -0.9961177865
H -4.7120248986 -0.7421993906 -0.4658968881
H -3.9731939591 1.4144072753 0.7422781578
H -2.5456559115 1.1871482611 1.7713309394
H -3.9779155477 0.1596329796 2.0300006787
H 0.9642196415 -1.5402753005 -1.4360777518
H -0.1787102969 -0.5169141315 -2.337110598
H -0.35937648 -2.2872343842 -2.3661189781

15_SCRF:
E_{tot}= -858.398616

N 0.484656058 2.7739342616 -0.7774449031
C 0.3478566282 1.5198954125 -0.4129858077
O -0.817942853 3.2389639624 -1.1191549572
C 1.5474425459 0.7854883342 0.0468382863
C 1.4897656552 -0.0647632557 1.1633235072
C 2.6331120725 -0.734367421 1.6006769684
C -1.0225408722 1.090184877 -0.4526694433
C 3.8481984466 -0.56074746 0.9322053549
C -1.5943251462 -0.195825081 -0.249444035
C 3.9157765433 0.2908819169 -0.1738486233
C 2.7739526704 0.9597919446 -0.6149727517
C -1.7609200655 2.2405500335 -0.906809832
O -2.9446651847 2.4522738795 -1.151990823
N -2.8024249292 -0.3223858569 0.3516459971
N -0.9645922518 -1.3304059691 -0.6603561024
C -1.0471142143 -2.5913302819 0.0770516791
C -3.7690671009 -1.3541002301 -0.0316922843
C -3.3209238577 0.6842653173 1.2779383672
C -0.074991302 -1.3619853683 -1.8200157819
H 0.5563719108 -0.1836423666 1.706939561
H 2.5757017965 -1.3860798126 2.4709770915
H 4.7389342909 -1.08577461 1.2734247739

H 4.8592450282 0.4314113923 -0.6988888677
H 2.8220022229 1.6153046992 -1.4815297088
H -1.6007144238 -3.3564280495 -0.480386344
H -1.5264388265 -2.4308759686 1.0433070629
H -0.0286539193 -2.9583335845 0.2505209423
H -3.9257885307 -2.0835570317 0.7714331113
H -3.4319922387 -1.8704129796 -0.9304941558
H -4.7257090063 -0.8658790605 -0.2492751681
H -3.9711621434 1.3944728144 0.7577432065
H -2.4914410939 1.2290629667 1.7306366362
H -3.8833627674 0.1710013441 2.0647504621
H 0.9722579603 -1.4633253144 -1.5157810255
H -0.1932743004 -0.4500020975 -2.404818337
H -0.3453028019 -2.2219283564 -2.4443980561

15_rot_ts:
E_{tot}=-858.347203189 (-64.9 cm^{-1})

N -0.8146236085 2.3295225916 -0.2794626128
C -0.2424036323 1.2734637491 -0.8250492001
O -0.134048226 2.5721054236 0.9251481611
C -0.7464707257 0.7806389389 -2.1235732409
C -0.5538872631 -0.5479396172 -2.5333647754
C -1.0391997086 -0.9954830056 -3.7629475114
C 0.8284175387 0.78314222 -0.023569588
C -1.7296181309 -0.1221851786 -4.6036368393
C 1.8077688063 -0.2722008238 -0.2219406836
C -1.9335392293 1.2016427744 -4.2029663725
C -1.4456230106 1.6509401194 -2.9790345257
C 0.8818430687 1.6358091957 1.1211097899
O 1.5763095088 1.627157279 2.1354324101
N 2.8847915847 -0.0678200028 -1.0094424502
N 1.6682842957 -1.4388813003 0.4400796459
C 2.2077297368 -2.7247080845 -0.0088241094
C 4.1875335938 -0.7070496202 -0.7950163855
C 2.9394405748 1.0942780726 -1.9077596641
C 0.7350120257 -1.5183910952 1.5793264848
H -0.0457376665 -1.2466410904 -1.8740073193
H -0.8850924981 -2.0301086082 -4.0593802061
H -2.1078533423 -0.4692677534 -5.5615035383
H -2.4721197035 1.8884975823 -4.8507471233
H -1.5978457404 2.6767935203 -2.6605580061
H 3.0274582462 -3.0827661412 0.6245088796
H 2.5487276466 -2.6557971978 -1.0416399071
H 1.3970476599 -3.4598296549 0.0329069172
H 4.4322143246 -1.4367386067 -1.575261473
H 4.2185599072 -1.1863766969 0.1824545407
H 4.9495796854 0.0785325369 -0.8074555034
H 3.3563860049 1.9636813875 -1.3870658368
H 1.9495891382 1.3394264652 -2.2821092732

H 3.5840042437 0.8356967351 -2.7532445307
H -0.2937183947 -1.6693575154 1.2354015301
H 0.8075586415 -0.610915713 2.1784387098
H 1.0390839682 -2.3723249856 2.1911794872

16:
E_{tot}= -1010.8043726

N -3.3564476279 0.1227217275 0.7393580009
C -2.1025829837 0.2427791659 0.3850885771
O -3.5979246561 -1.2436687603 0.9917899727
C -1.6158413812 1.5860842897 0.0017647038
C -2.1087004171 2.7210494903 0.6661321106
C -1.6861242722 3.9964113436 0.2969959531
C -1.4353996924 -1.0372087962 0.3370280271
C -0.7638311684 4.1605908677 -0.7394413034
C -0.0952745931 -1.3878576215 0.1434264584
C -0.2739906328 3.0388580026 -1.4112307395
C -0.697548372 1.7610394888 -1.0454568974
C -2.4621493782 -2.0017459254 0.7206251251
O -2.4527723153 -3.2056193874 0.8717594963
N 0.9540833759 -0.5927560436 0.5194515757
N 0.2641575367 -2.592633487 -0.401187499
C -0.4364789983 -3.4067781074 -1.328422083
C 0.8771884018 0.315593092 1.6592587979
C 2.2656639071 -0.6710735125 -0.1131874286
C -0.2022374249 -4.7854162709 -1.2970883595
C -0.800845397 -5.6182381462 -2.2399230664
C -1.6434943944 -5.0857036607 -3.2159342632
C -1.8741166995 -3.7088421232 -3.2434751909
C -1.2688611518 -2.8652898466 -2.3147295305
H -2.8266301623 2.5856108203 1.4685528567
H -2.0757882994 4.8646522471 0.82174348
H -0.4325762824 5.15559786 -1.0243004304
H 0.4310271863 3.1587187704 -2.2298763437
H -0.3296551813 0.8952586034 -1.5878212286
H 1.1160008805 -3.0024061351 -0.0388541598
H 1.7190324435 0.1125664565 2.3342967848
H -0.0548643314 0.1506337627 2.1983547707
H 0.9246887336 1.3619958799 1.3400429897
H 2.6433316536 0.3448829873 -0.2782714766
H 2.1892171964 -1.1747602417 -1.0780491676
H 2.9958217503 -1.2033221227 0.514268366
H 0.4328891742 -5.2058504413 -0.5208680193
H -0.6149199653 -6.6879157861 -2.2008671705
H -2.1176842534 -5.7355712117 -3.945462331
H -2.5255967964 -3.2808099404 -4.0003202912
H -1.4482534114 -1.7967062879 -2.3504500666

16_SCRF:

E_{tot}= -1010.8350887

N -3.3740625578 0.083237838 0.7307365845
C -2.1113359299 0.1932584957 0.3876009591
O -3.5955399312 -1.288462696 1.0345214226
C -1.6169469758 1.5241781235 -0.0317876369
C -2.0580047123 2.6766168382 0.6393954659
C -1.6251605859 3.9392912549 0.2351154517
C -1.4359674746 -1.0762097039 0.4024109167
C -0.745089361 4.0690385942 -0.8429123749
C -0.0732869236 -1.4088330467 0.2029039721
C -0.3046983481 2.9281399112 -1.5191623607
C -0.7378058622 1.6638849683 -1.1179414798
C -2.4392919115 -2.0299222082 0.8122329214
O -2.4330768772 -3.2346440163 1.0233286198
N 0.9406958707 -0.594317305 0.5849434569
N 0.2914137715 -2.5951238934 -0.3643735002
C -0.4198006298 -3.3720913358 -1.3177817057
C 0.8331036494 0.3292403611 1.7139794123
C 2.2602166523 -0.6268582324 -0.0468825197
C -0.1805394038 -4.7508844679 -1.3519684267
C -0.79710919 -5.5456939874 -2.3176592623
C -1.6641777827 -4.976113599 -3.2523516852
C -1.897738519 -3.5986273133 -3.217772637
C -1.2742347184 -2.7934438184 -2.2655562431
H -2.7345835735 2.5731116114 1.4846367689
H -1.9716224115 4.8236145748 0.76757012
H -0.4040325504 5.0547711042 -1.1552447239
H 0.3726982695 3.0211412099 -2.3664436753
H -0.4047428721 0.7863205503 -1.6647577295
H 1.1457639453 -3.0244990058 -0.0078626374
H 1.6783544973 0.1522472156 2.3899041435
H -0.0957300316 0.1512790609 2.2542787021
H 0.8632851433 1.369337008 1.3751574502
H 2.5983829549 0.4041518418 -0.1966232213
H 2.201192926 -1.1244661645 -1.0160595148
H 2.9967858576 -1.1442571606 0.5816545798
H 0.4892807183 -5.1979919888 -0.6177275102
H -0.5998751985 -6.6163172201 -2.3321697971
H -2.1489127714 -5.5969214393 -4.0033731868
H -2.5616834055 -3.1378552759 -3.9473720799
H -1.4536117467 -1.7244556833 -2.2618660392

16_rot_ts:
E_{tot}=-1010.7878015 (-75.3 cm^{-1})

N 0.5331983488 -2.5343556602 -0.1148663682
C 0.4349038899 -1.3235984451 0.3970723612
O -0.0887843518 -2.4892050982 -1.3754779692
C 1.0483814442 -1.0541394522 1.714114584

C 2.0960972543 -1.8720804066 2.1728750714
C 2.6907406358 -1.6365356699 3.4093019884
C -0.2497793454 -0.437868386 -0.4884616295
C 2.2588930682 -0.5761105789 4.2113547992
C -0.4453793727 0.9955969062 -0.4518495236
C 1.2180764419 0.2397562309 3.7677586796
C 0.6162912513 0.0013420865 2.5312603923
C -0.5714919409 -1.210663372 -1.6455095288
O -1.1656480277 -0.9442131287 -2.6884702238
N 0.46704967 1.8414754287 -0.9596935667
N -1.5743260229 1.539036191 0.0516140309
C -2.767338125 0.8443012761 0.4469536641
C 1.7732605567 1.3856568206 -1.4472568055
C 0.2193881662 3.2809331843 -1.0570551784
C -3.3721992824 -0.0864331999 -0.4021089542
C -4.5574317575 -0.6963393607 0.0085827345
C -5.1456306192 -0.3650972989 1.2314412677
C -4.5429370106 0.5829114602 2.0593732814
C -3.3480645109 1.1883826014 1.6704185122
H 2.4281303137 -2.6902347089 1.5425474025
H 3.4991663653 -2.279724392 3.7474113302
H 2.7276897824 -0.3908054076 5.1742047246
H 0.8646879889 1.0585956521 4.389787206
H -0.2167597576 0.6216303076 2.2153209133
H -1.6223272914 2.5453077566 0.1563996803
H 1.8681602419 1.6266199311 -2.5109003763
H 1.8549105 0.3105959614 -1.3126010056
H 2.5684341085 1.8901246933 -0.8879140871
H 0.9999634487 3.7314671951 -1.6706454629
H 0.2410704639 3.7647979923 -0.0710968651
H -0.7452683661 3.4733063008 -1.539786124
H -2.9236606441 -0.3232679968 -1.3634698317
H -5.0265375909 -1.4288177452 -0.6417133625
H -6.0726939871 -0.8419435641 1.5367311165
H -4.9939378386 0.8469529804 3.0115875882
H -2.8625023376 1.9142093751 2.3184926143

17:
E$_{tot}$= -857.1798172

N -0.6894469585 2.521517283 -0.1926004268
C -0.6110596335 1.2178183273 -0.0876896402
O 0.6187719616 3.0297036104 -0.0566782976
C -1.8684735115 0.4401615736 -0.132399442
C -2.9262522271 0.8721795612 -0.9492276079
C -4.1276129973 0.1676453914 -0.9824443287
C 0.7372111802 0.7836219283 0.1746598388
C -4.2932883412 -0.9806995254 -0.2039459191
C 1.3214525724 -0.4964786538 0.2232274778
C -3.2501930815 -1.4138823674 0.6167043992

C -2.0474489992 -0.7078777513 0.6549639152
C 1.5227685542 2.0043901001 0.1954798044
O 2.7147265252 2.2286263139 0.3238645917
N 0.973826881 -1.5768261885 -0.5332735651
N 2.3536473044 -0.8335073361 1.0335554927
C 2.8881907311 -2.1518424749 0.6952140654
C 1.7531123103 -2.7569362371 -0.1521380023
C 0.1904819938 -1.555686955 -1.7543658034
C 2.881213987 -0.0457290861 2.1345334552
H -2.7902007588 1.7657641289 -1.5496961045
H -4.9364803305 0.5140843347 -1.6203076586
H -5.2297804466 -1.5312416332 -0.2335367245
H -3.3762399547 -2.2969999157 1.2379155197
H -1.2497286268 -1.0356530253 1.3149962526
H 3.8282116779 -2.0621020488 0.1329286961
H 3.087373964 -2.7265493442 1.6046750429
H 1.1386616865 -3.4663722285 0.4194762578
H 2.1228739982 -3.2704279456 -1.0449167087
H 0.747629499 -2.062099093 -2.5523762508
H 0.0138284701 -0.5215071664 -2.0509796832
H -0.7770068833 -2.0525239802 -1.6241903853
H 3.1856913647 -0.7290771232 2.9347318853
H 2.094907258 0.614210379 2.5052805014
H 3.7225058307 0.5765011481 1.8201123525

17_SCRF:
E$_{tot}$= -857.2062298

N -0.6888017704 2.5604401445 -0.1568363621
C -0.5913410877 1.2508840923 -0.0732085624
O 0.6377784224 3.064808228 -0.0600158068
C -1.8347843742 0.4486607642 -0.1004638547
C -2.8861637015 0.8144801973 -0.9570627657
C -4.070944773 0.0791428633 -0.9750213705
C 0.7610887885 0.8234606083 0.1238498752
C -4.221731843 -1.0319688323 -0.1404068946
C 1.3287735826 -0.4855810617 0.1769824693
C -3.1826718466 -1.3995397476 0.7186933874
C -1.9971056147 -0.6635841008 0.7413961567
C 1.5432392534 2.0265096545 0.1333957966
O 2.7455053616 2.266375781 0.2243000785
N 1.0145591712 -1.5202048947 -0.6299872916
N 2.289346676 -0.8527303534 1.0452525889
C 2.8004514139 -2.1953002615 0.7347692808
C 1.7239071221 -2.741482164 -0.2202475749
C 0.2033219939 -1.4873359059 -1.8327519236
C 2.8009164718 -0.0739744818 2.1590318098
H -2.7628077724 1.6730699713 -1.6130413058
H -4.8763882524 0.3711905137 -1.6470198815
H -5.1453652211 -1.6082548176 -0.1583139888

H -3.2966717954 -2.2569821636 1.379930718
H -1.2064883448 -0.9423004883 1.4335401274
H 3.7887022154 -2.1268457501 0.2610352487
H 2.8911317802 -2.7855485975 1.6511229419
H 1.0328515096 -3.4350371825 0.2767553183
H 2.1496589702 -3.2401339558 -1.0958688325
H 0.7381797663 -2.0063466289 -2.6359086675
H 0.0349289677 -0.4519538948 -2.1305074206
H -0.7646570859 -1.9755396438 -1.6755409705
H 3.0186517987 -0.7548171386 2.987630867
H 2.0412771272 0.6433254999 2.4743809617
H 3.7055280902 0.475317747 1.881688848

17_rot_ts:
E_{tot}=-857.1628307 (-77.2 cm^{-1})

N 0.3987587057 3.0154226591 0.5862151612
C 1.1311196337 1.962114331 0.8856034082
O -0.4241059709 2.6472196432 -0.4911162614
C 2.1211115312 2.0690404054 1.9777074691
C 2.724986414 0.9389611678 2.5487422776
C 3.6604983245 1.0681187099 3.5767072686
C 0.8215779525 0.8582501954 0.034238414
C 4.0065328649 2.3309796471 4.05591414
C 1.3632202092 -0.4647463554 -0.1073188154
C 3.4067727974 3.4644988375 3.4983545334
C 2.4779123344 3.3374688262 2.4702741925
C -0.1881946158 1.3230287995 -0.8738490398
O -0.7834383557 0.7957604783 -1.8031898213
N 2.3464329871 -0.8040849341 -0.9536931258
N 0.9050589837 -1.5595873137 0.5271141173
C 1.5454902712 -2.7831188542 0.0363713218
C 2.6380356961 -2.239114248 -0.9152166002
C 3.0927185175 0.1056966504 -1.8015666638
C -0.2651471987 -1.6072009286 1.3843497357
H 2.452250981 -0.0544686442 2.2050145005
H 4.1139246663 0.1783302002 4.0067308561
H 4.7348611346 2.4329710521 4.8560392307
H 3.668962354 4.4537538691 3.864604483
H 2.0123643729 4.2126581857 2.029979486
H 1.9577063518 -3.3661162919 0.8663958001
H 0.8069871324 -3.4041584865 -0.4852309042
H 2.5774175554 -2.6689524249 -1.9203448331
H 3.651926507 -2.4066194286 -0.5314455209
H 4.1576931621 0.0805224234 -1.5416710552
H 2.7009522332 1.1118677116 -1.6517744097
H 2.9726529743 -0.1787325084 -2.8526547308
H -1.065664805 -2.1800341742 0.9009108398
H -0.6057046033 -0.5852568498 1.5540794467
H -0.0137600984 -2.0785753506 2.340749099

18:

E_{tot}= -1015.6385389

N 2.0533135106 3.098776634 0.334043811
C 1.5780876351 1.9007829937 0.1065676214
O 1.2188005811 3.7017436255 1.3015917721
C 2.2421706618 1.0867261582 -0.9358578319
C 3.6346434475 1.1676944753 -1.0991488408
C 4.2738332558 0.4407524382 -2.1024401856
C 0.3760561301 1.645855803 0.8638200305
C 3.5329931715 -0.3749777907 -2.9607496017
C -0.3238303598 0.4459712781 1.067573939
C 2.1466254017 -0.4529656258 -2.8125739595
C 1.5058210522 0.2710690997 -1.8082886421
C 0.1511620637 2.8720159532 1.6114311534
O -0.6985744073 3.2251168023 2.4118911446
N -1.6643627298 0.3608136397 1.2762555458
N 0.3115944722 -0.7783294051 1.0570002628
C -2.8532173548 1.1380962172 0.8098185851
C 1.4353432266 -1.2814101321 1.9155044643
C -2.4992315228 2.2011059628 -0.2355332151
C -3.5275727666 1.7767243593 2.0368743165
C -3.7963934132 0.0972615284 0.1695601356
C 0.8006149815 -2.2168954361 2.9681433724
C 2.1871381198 -0.1598757867 2.640306163
C 2.3930388963 -2.0839629326 1.0189456351
H 4.2028011057 1.810598781 -0.4344906299
H 5.3525372101 0.5119735294 -2.2139757971
H 4.0316722668 -0.9426964279 -3.7417979302
H 1.5613534323 -1.0750971354 -3.484866418
H 0.4264577016 0.216199175 -1.7083008865
H -1.94092053 -0.4829015718 1.7660066049
H -0.3141468678 -1.5396093913 0.8111744058
H -1.9253205409 1.7797463828 -1.0671064992
H -1.9427282134 3.0298776064 0.2002743443
H -3.4348826122 2.600556847 -0.6415375281
H -2.8319610852 2.4613226284 2.5251939393
H -3.8365052562 1.00682833 2.7555074884
H -4.4255137088 2.3251239882 1.7299099827
H -4.049095196 -0.7028805075 0.8778679733
H -3.3417545608 -0.3580326906 -0.717802226
H -4.73460573 0.5742678844 -0.1318757117
H 0.2435287488 -3.0336040341 2.4901619208
H 0.1153818907 -1.6651593007 3.6219419817
H 1.5744348894 -2.6722195632 3.595522764
H 1.5183639734 0.4482251332 3.2566846318
H 2.7169747171 0.500124425 1.9519492466
H 2.9289545564 -0.621197546 3.3012956545
H 2.8596309215 -1.4399483326 0.270268481

H 1.860182835 -2.8865515023 0.4942634504
H 3.1802619992 -2.5463015669 1.6249810814

18_SCRF:
E$_{tot}$= -1015.6614403

N 0.2366996983 1.7939652257 1.4996114256
C 0.9940222709 1.7154518806 0.4181830838
O 0.9877997686 1.2293302435 2.558302015
C 0.3757605447 2.1042789981 -0.8749842673
C 1.1100822955 2.2019978015 -2.0677646944
C 0.4858094964 2.5484487694 -3.2685168905
C 2.249721799 1.0934964025 0.7038010565
C -0.8844634122 2.8059437351 -3.302205049
C 3.4282175435 0.8398278042 -0.1005211163
C -1.6299404404 2.7045358491 -2.1225810558
C -1.011032894 2.3513166769 -0.9271216876
C 2.204349731 0.7453057501 2.086760536
O 2.9894255883 0.2012762308 2.8681663578
N 3.8493292761 -0.4006536172 -0.3854331347
N 4.191064187 1.8467661512 -0.5833218693
C 3.1621270267 -1.7331004751 -0.3388469732
C 4.439263626 3.2273864891 -0.04017015
C 1.629752255 -1.6465733425 -0.3400827205
C 3.6696552302 -2.484839396 0.9042067971
C 3.596478773 -2.4644487759 -1.6237115837
C 5.9458233817 3.4810550779 -0.2494654849
C 4.1324502397 3.3468869291 1.4610843013
C 3.6277756218 4.2621657464 -0.8362714473
H 2.1765435558 2.0118899094 -2.0702518325
H 1.0792812595 2.6177395323 -4.1787741046
H -1.370238804 3.0767386376 -4.2382300861
H -2.7027730602 2.8909049605 -2.1365579167
H -1.5980359128 2.2572495122 -0.0186201543
H 4.8206688044 -0.4720265131 -0.7054847584
H 4.8545857957 1.5748585811 -1.3136713986
H 1.2632208972 -1.0078116522 -1.1495830486
H 1.2194272949 -1.2855962914 0.6024573843
H 1.244574369 -2.658413756 -0.5073521205
H 3.4183069892 -1.9270478969 1.8099202395
H 4.7583568233 -2.6103448454 0.8630929069
H 3.2164143436 -3.481364331 0.9496601751
H 4.6895664242 -2.5305522521 -1.696758979
H 3.2223614038 -1.9510952935 -2.5165067799
H 3.2015805438 -3.4850971995 -1.6208323467
H 6.2229178876 3.3886226386 -1.3075091463
H 6.5475376374 2.7725323847 0.3305352732
H 6.198963322 4.4949730359 0.0741723878
H 4.5780804289 2.5264468542 2.0324991551
H 3.0615842411 3.3710964117 1.6671764884

H 4.5642863653 4.2881523472 1.8180386967
H 2.5531632534 4.1140560298 -0.7038497529
H 3.8540547681 4.2046001095 -1.9069834782
H 3.8793787617 5.270956932 -0.4894492523

18_rot_ts:
E_{tot}=-1015.62577 (-106.3 cm^{-1})

N 0.7396738181 -2.1835739349 -1.367028982
C 0.6515227527 -1.3309149507 -0.3627730413
O -0.5645484351 -2.3720258713 -1.8519458272
C 1.897073891 -0.953096916 0.3417627099
C 3.0679007697 -1.7032050137 0.1240945235
C 4.2572005253 -1.3670293977 0.7631038785
C -0.6988410428 -0.9273464511 -0.1466295508
C 4.3082243204 -0.2788011381 1.6397432978
C -1.3225806914 -0.0455605707 0.8202678445
C 3.1550991167 0.4712604134 1.8658663761
C 1.9613788267 0.1381149029 1.2226119166
C -1.4794623196 -1.6125359696 -1.1243757638
O -2.6822303398 -1.6264634113 -1.3825571364
N -1.8065810925 -0.4976261302 1.9858886605
N -1.4855440375 1.2721598436 0.5905154946
C -1.7550192214 -1.8512190147 2.6389389001
C -1.4484650188 2.0631716638 -0.690453543
C -2.1560502734 -2.9839937291 1.6775464745
C -2.7956258008 -1.7595595616 3.7713918123
C -0.3565282921 -2.0917937062 3.2287083219
C -2.712350077 1.7420591744 -1.5086820926
C -0.1730459611 1.8159621319 -1.5097878292
C -1.4676032958 3.5332812627 -0.2317633084
H 3.0218161002 -2.54740691 -0.5552161771
H 5.1497500318 -1.9597004768 0.5798232401
H 5.2376567701 -0.0201983682 2.1400335853
H 3.1815086185 1.3227285408 2.5413993392
H 1.0804611517 0.7463282315 1.4003372243
H -2.2794815251 0.1891710227 2.566093736
H -1.9787952061 1.781807159 1.319119876
H -1.3343023816 -3.2708568186 1.020887559
H -3.0036913227 -2.6968294935 1.0498144588
H -2.4362792681 -3.860764154 2.2724325951
H -3.8047711671 -1.6104437366 3.3705371383
H -2.5657459555 -0.941616113 4.467513538
H -2.7954680504 -2.6888346233 4.3473667278
H -0.0867160488 -1.3096438711 3.9476019306
H 0.4033688716 -2.1171297535 2.4446668903
H -0.3409804363 -3.0550827184 3.7505336709
H -3.615756107 2.0316785105 -0.9576333742
H -2.7808083902 0.6743911496 -1.7376288532
H -2.6969037682 2.3078258281 -2.4472224244

H -0.16099566 0.8296676673 -1.9716799682
H 0.7240787026 1.9216981939 -0.8921547823
H -0.1289493657 2.5677382567 -2.3057937915
H -0.5719166679 3.7825475036 0.3483625744
H -2.3543001817 3.7553205904 0.3774369146
H -1.5015746059 4.190368837 -1.105287764

19 (minimum 1)**:**
E$_{tot}$= -1093.0392919

N -1.2275103484 -2.2500272855 -1.5958321299
C -1.0587440241 -1.3051606094 -0.7011777316
O -0.0220833515 -2.3429034233 -2.3205646573
C -2.1679675118 -1.0266982687 0.237770636
C -1.933407192 -0.5816907013 1.5482483764
C -2.9962123653 -0.3453657534 2.4207187514
C 0.2724903429 -0.7689458446 -0.7345758699
C -4.3110795119 -0.5512422482 1.9996082427
C 0.8129840362 0.3380057133 -0.0281610028
C -4.5549014433 -1.0031757423 0.7002704664
C -3.4953658124 -1.2382389346 -0.1730680156
C 0.9371913965 -1.4849174614 -1.7933112713
O 2.0610597022 -1.4312416826 -2.2765293457
N 0.1882384281 1.5606535228 0.0608433539
N 1.963157674 0.3435745682 0.7067954192
C 2.2607986827 1.7315048254 1.1117757999
C 0.8700555449 2.3416170456 1.110088223
C -0.5729672933 2.3349601651 -0.9916981365
C 2.9378599264 -0.7560901725 1.0532076005
C -1.6765707007 3.1246439916 -0.2616392753
C 0.4088298132 3.2907227463 -1.7121824593
C -1.2364768229 1.4697275388 -2.0726650734
C 2.3006772724 -2.1566966349 1.0117173196
C 3.4333245134 -0.5298347183 2.5011539324
C 4.1260837363 -0.6767137859 0.0759043088
H -0.9139166664 -0.4431666334 1.895448321
H -2.7954933609 -0.0085658298 3.4346804254
H -5.1384649547 -0.3653287253 2.6792324827
H -5.5748934422 -1.1714717863 0.3647585793
H -3.6773114327 -1.5940032143 -1.1820352448
H 2.9321367196 2.2099764845 0.3848388121
H 2.7219559684 1.7729961532 2.0950624124
H 0.8747135696 3.4071983609 0.8931954301
H 0.3639868352 2.1867917483 2.0728250698
H -1.2742009899 3.83191928 0.4714682544
H -2.3543191078 2.4392221871 0.2563381422
H -2.256917757 3.7026860244 -0.988093143
H 1.1995440202 2.7209963464 -2.2118174816
H 0.8758042952 4.0174939331 -1.0397080812
H -0.1296575325 3.8620431246 -2.4756358952

H -1.997472346 0.805490565 -1.6645678201
H -0.5159893372 0.8792125605 -2.6402866003
H -1.7331731834 2.1538716028 -2.7697375319
H 2.130178518 -2.5065345766 -0.0029714843
H 1.3621068705 -2.1966485478 1.5724882177
H 3.0038084626 -2.8515881649 1.4829647989
H 2.5970238974 -0.4542779916 3.2060580026
H 4.0668461131 0.3561522122 2.6052241569
H 4.043722816 -1.3875636326 2.7970906715
H 4.6266872161 0.2972379594 0.1401629473
H 3.7778769628 -0.8426922724 -0.9463007416
H 4.8650988755 -1.4451676001 0.3302514693

19 (minimum 1) **SCRF**:
E$_{tot}$= -1093.0655699

N -1.0870828472 -2.2937073781 -1.6180281024
C -0.9440105306 -1.3300440261 -0.7275332317
O 0.0981232605 -2.268821504 -2.4071472387
C -2.033291206 -1.1047021844 0.2495844579
C -1.7701075227 -0.6692302565 1.558600665
C -2.8117127312 -0.4733074804 2.4666662074
C 0.3141276683 -0.6741365761 -0.8457333856
C -4.1329451379 -0.7133141614 2.0821082607
C 0.8336781534 0.4376285711 -0.0778841905
C -4.4051919542 -1.15311237 0.7841516769
C -3.3655820873 -1.3454198262 -0.1255026901
C 0.9797297273 -1.2973312041 -1.9350119431
O 2.064159525 -1.1258110377 -2.502680776
N 0.2938100899 1.6786252815 -0.0764482294
N 1.8905701261 0.3604979251 0.7636093616
C 2.2474667009 1.7303518156 1.2061097437
C 0.9391593635 2.4723328832 0.9954227385
C -0.5611004007 2.4190733437 -1.0789942972
C 2.7944718388 -0.7971595307 1.125531673
C -1.606217065 3.2227676652 -0.2792906292
C 0.3632120278 3.3576361336 -1.8855395991
C -1.3058531626 1.5221397177 -2.0754978743
C 2.078035392 -2.1589312332 1.0854603539
C 3.2859127258 -0.5866204213 2.5744339351
C 3.9965711088 -0.7922722257 0.1614337787
H -0.746430556 -0.5013850234 1.8797145435
H -2.5883585277 -0.140154245 3.4784472436
H -4.9449657295 -0.5600540778 2.7903993481
H -5.4316008593 -1.3427039441 0.4758226849
H -3.5772364232 -1.6823179114 -1.1369901736
H 3.0627011914 2.1229262932 0.5836392635
H 2.5561735708 1.749087645 2.248395203
H 1.0907398908 3.5090576859 0.700279704
H 0.3080735585 2.4503202071 1.892899202

H -1.1508404845 3.9506360047 0.3993683657
H -2.2406515379 2.5499892674 0.3068455978
H -2.2434002654 3.7779109512 -0.9749943378
H 1.1044982705 2.7768998076 -2.4448016064
H 0.8914206918 4.0802576704 -1.2558725776
H -0.2352492671 3.9276399785 -2.6040564803
H -2.0082734708 0.851462467 -1.5808078368
H -0.630738849 0.9370957667 -2.7014256203
H -1.8816230344 2.1850698205 -2.7306315884
H 1.8709283355 -2.5055393059 0.0755656774
H 1.141809723 -2.1435396216 1.6521631391
H 2.7417425448 -2.8919450803 1.5558560941
H 2.4489168161 -0.4742628377 3.2731987288
H 3.9511210962 0.275601391 2.6752240382
H 3.8594186849 -1.4680288599 2.8749223306
H 4.5578164765 0.1469478651 0.232710406
H 3.6560767664 -0.9280398796 -0.8688045326
H 4.6811440462 -1.6073175379 0.4227441496

19 (minimum 2):
E$_{tot}$= -1093.0389069

N -0.8576985134 -2.3789482071 -1.4391730759
C -0.4763393325 -1.7213467014 -0.3597461425
O -0.0379017649 -1.9383674932 -2.4903938628
C -1.181357956 -1.9941377426 0.9120274966
C -0.8479199959 -1.3448267957 2.1110170867
C -1.5335263565 -1.6253422303 3.2950218006
C 0.5972094954 -0.8313598792 -0.6518425648
C -2.5664081935 -2.5609361448 3.3035547552
C 1.3582307666 0.0933548235 0.1593411567
C -2.9082680345 -3.214781193 2.1153194093
C -2.2266248288 -2.9367214108 0.9353088573
C 0.871527808 -0.9831117803 -2.0402309749
O 1.6893895721 -0.4605775017 -2.8013218188
N 1.0363608115 1.3929220547 0.3329841138
N 2.5034778261 -0.2240410179 0.7999008011
C 3.1037566768 0.9766147765 1.4059128747
C 2.0943857744 2.0889915241 1.0847932675
C 0.001762672 2.2162210332 -0.4026472595
C 3.3481919062 -1.4717704144 0.6620519136
C -0.291922495 3.4675451048 0.4514750331
C 0.5959549857 2.6253949933 -1.7643075586
C -1.3335425545 1.4725844124 -0.5889982231
C 2.5095753649 -2.7627673053 0.6337916045
C 4.2645744256 -1.553853322 1.9010418459
C 4.1926823926 -1.3385451174 -0.6200140971
H -0.047629254 -0.6124869152 2.1299545775
H -1.2566608262 -1.1091896405 4.2110005323
H -3.1006387511 -2.78007794 4.2242073797

H -3.7121101319 -3.9464444633 2.1097248098
H -2.4876319291 -3.4407980929 0.0112754322
H 4.087088739 1.1738289577 0.9673921854
H 3.2333170862 0.8400007696 2.4825770776
H 2.5366829316 2.8825643456 0.4742619117
H 1.6860847368 2.5449044275 1.9903820691
H 0.5830105821 4.1095016062 0.5901749744
H -0.6924953202 3.197238198 1.4352459595
H -1.0488373043 4.0659260061 -0.0632609344
H 0.878419505 1.7465799536 -2.3518788399
H 1.4847279701 3.2558300755 -1.6373348621
H -0.1422871025 3.2076206046 -2.3269754773
H -1.6705534301 1.0167736409 0.3468417366
H -1.2864784014 0.6998165605 -1.3531883856
H -2.0852643749 2.2076626979 -0.8972910108
H 1.9904262769 -2.9116121629 -0.3105095864
H 1.7726776827 -2.7778237081 1.4424264793
H 3.1914518026 -3.6075564422 0.7815974415
H 3.6824439277 -1.6240255944 2.8270706606
H 4.956725736 -0.7104695297 1.9815530374
H 4.8723840554 -2.4593924806 1.8204229191
H 4.8790161235 -0.4850085838 -0.5575045192
H 3.5561211603 -1.204622852 -1.4998977636
H 4.8007855877 -2.2400612236 -0.7544072828

19 (minimum 2) **SCRF**:
E_{tot}= -1093.066938

N -0.867223646 -2.3889867311 -1.4632404949
C -0.4667571593 -1.7195028256 -0.3936906127
O -0.0531181727 -1.9484209998 -2.5313369739
C -1.1555993006 -1.9810837213 0.8923648751
C -0.8051303601 -1.3181080084 2.0796613318
C -1.4733510004 -1.5855430592 3.2767356841
C 0.603293722 -0.8339396892 -0.7053968684
C -2.5064398699 -2.5220007099 3.3104320916
C 1.3671235309 0.0943304891 0.1201594639
C -2.8661317076 -3.1898327034 2.1348512046
C -2.2000922479 -2.9236948216 0.9416704964
C 0.8589501588 -0.9907805293 -2.0894033368
O 1.6609952386 -0.4836302641 -2.8857791096
N 1.0350370014 1.3856993289 0.3030849633
N 2.4984420615 -0.2333744969 0.7720696493
C 3.0791480187 0.9608759881 1.4206423779
C 2.0749659775 2.0746927446 1.0954768744
C -0.0093723032 2.2184246193 -0.4062715436
C 3.3403371009 -1.4858738986 0.667356005
C -0.3072535875 3.4477583183 0.4772586076
C 0.5768005276 2.6660780549 -1.7593382044
C -1.3405530295 1.471972296 -0.606744076

C 2.501372638 -2.7759454219 0.63437725
C 4.2322693574 -1.5574461469 1.9240447334
C 4.2141576445 -1.3693619673 -0.5956195925
H -0.0070148957 -0.5849463734 2.0843139176
H -1.1817100285 -1.0573100933 4.1830054497
H -3.0281661025 -2.7312763778 4.2428273881
H -3.6710401684 -3.9230920892 2.1483725369
H -2.4835785771 -3.4452978181 0.0318990225
H 4.0729834335 1.1691954014 1.0118934424
H 3.1743738407 0.8005974044 2.4972140375
H 2.5275509091 2.8804471919 0.5089757785
H 1.6389232798 2.5077571379 1.9990665024
H 0.5664152732 4.0879314259 0.6271515858
H -0.7009965068 3.151849038 1.4560974416
H -1.0694916743 4.0519379089 -0.0231628112
H 0.8365809399 1.8025228956 -2.3785370416
H 1.4775423082 3.2749392962 -1.6188622962
H -0.1582362874 3.2779250412 -2.2941292917
H -1.6793130068 1.0053324957 0.3231305941
H -1.2884246377 0.7089883037 -1.3813582524
H -2.0936086799 2.2073679729 -0.9094989595
H 1.9927971024 -2.9287154609 -0.3157884228
H 1.7576128179 -2.7881797562 1.4367532501
H 3.1811227209 -3.6202981469 0.7911104021
H 3.6322028348 -1.6124479815 2.8393135188
H 4.9242447258 -0.7147750353 2.0054611762
H 4.8365767479 -2.4671103959 1.8632557235
H 4.8825110966 -0.5024136252 -0.5362628709
H 3.5958972516 -1.2680965461 -1.4926513151
H 4.83872222 -2.2642649782 -0.6942283423

10:
E$_{tot}$=-839.2262807

O -0.4999791746 0.9472651052 1.2638103308
C -0.4023289709 1.7057740665 0.3119211231
O -1.4599079325 2.5496863894 0.053563131
C -1.2606625182 3.6717163605 -0.8124972022
O -0.5209431905 3.3154813612 -1.9838133275
C -0.5369837349 4.7920942305 -0.0609369572
C 0.6893687884 1.7521928462 -0.6387398677
C -2.6432640153 4.082130698 -1.2943484971
C 1.8155885881 0.8989278606 -0.4223496951
C 0.6101383379 2.5357024448 -1.8531899875
O 1.4283958408 2.5680602858 -2.7578753356
N 2.3735873544 0.0776067344 -1.3400180568
N 2.4946390956 0.7894375881 0.7437740158
C 3.456145163 -0.3119397734 0.6870820892
C 3.6115361765 -0.5128993262 -0.8285310535
C 1.8656589268 -0.2328376843 -2.6631275863

C 2.2460810826 1.5239039365 1.9676762526
H -1.1108768693 5.0784494926 0.8253488797
H -0.4233984669 5.6636936978 -0.7121743466
H 0.4580431964 4.4664715703 0.2563390087
H -3.2692186709 4.361312079 -0.4421321324
H -3.1090688986 3.2439215055 -1.8187548845
H -2.5644857917 4.9316673253 -1.978421028
H 3.0537097288 -1.2049048113 1.1868610439
H 4.3919975209 -0.030589157 1.1777724188
H 4.4882630023 0.0151928221 -1.2294602911
H 3.6803493002 -1.5660944885 -1.1139706333
H 0.7857651883 -0.0782514383 -2.6759078161
H 2.0776032455 -1.2868156516 -2.8733627997
H 2.312418389 0.4058514573 -3.4292926875
H 1.8452617006 2.5077980539 1.7163846964
H 3.197220954 1.651754839 2.4947602721
H 1.520526654 1.0107495803 2.6057919236

10_rot_ts:
E_{tot}=-839.2135657 (-67.0 cm^{-1})

O -0.3333021509 1.0363881624 1.3997885653
C -0.2796349601 1.7777766658 0.4279066393
O -1.2464178556 2.7579224836 0.2868127597
C -1.0185253292 3.8228547604 -0.6464231238
O -0.4881263008 3.3552528062 -1.8941999926
C -0.0739870091 4.8604605271 -0.033866849
C 0.670795634 1.7080814224 -0.6382693226
C -2.3905946273 4.3968589655 -0.9662498995
C 1.6216487908 0.6055292203 -0.6096122907
C 0.5213971732 2.4087818823 -1.8758532307
O 1.1618229341 2.2141925053 -2.9000950561
N 1.36243061 -0.6331718955 -1.0394390459
N 2.8764933336 0.6841511566 -0.1513369568
C 3.582335293 -0.5951377576 -0.2567667048
C 2.5139280845 -1.5244674287 -0.882552553
C 0.1119196781 -1.1008668316 -1.6020728285
C 3.5177039316 1.8620029538 0.3942496094
H -0.4964997162 5.2441903425 0.8995220297
H 0.0704167071 5.6909027384 -0.7313569846
H 0.900357007 4.4144765487 0.1826544353
H -2.8642046208 4.7692227031 -0.0534089203
H -3.0192066769 3.6144740668 -1.3991698658
H -2.2969763165 5.2161513661 -1.6847453312
H 3.9062933126 -0.9316796419 0.7345392527
H 4.4703631904 -0.4865319038 -0.8896446127
H 2.819528704 -1.9230985708 -1.8564509445
H 2.2543592552 -2.3671957291 -0.2319847433
H -0.5932845118 -0.2708406727 -1.6203742079
H -0.2965000353 -1.9114933566 -0.9880845937

H 0.2721016252 -1.464458806 -2.6233601807
H 2.7999469368 2.6820371148 0.369861187
H 4.397346653 2.1265377204 -0.204235167
H 3.8301702562 1.6786964818 1.4289879274

20:
E$_{tot}$=-1714.9174108

N -0.0690424624 -3.4101106787 -0.862978806
C 0.1627101233 -2.283952131 -1.4831644617
O -0.2318772128 -3.1416355888 0.5057068866
C 0.2445542367 -2.3617633061 -2.9601467156
C -0.4301262315 -1.443646936 -3.7797034402
C -0.3992259337 -1.5756656922 -5.16350831
C 0.1576241949 -1.1548288733 -0.5637383732
C 0.3103550895 -2.6355148506 -5.7528097655
C 0.4762427282 0.186412869 -0.6847660084
C 0.9752037844 -3.5673759709 -4.9381697108
C 0.9376670198 -3.4291334041 -3.5557203018
C -0.1897599073 -1.7761214822 0.7281802936
O -0.3838614178 -1.3021402544 1.8242033978
S 1.3320057868 0.8611744786 -2.0902274626
S 0.0382237455 1.2596736982 0.6402262128
C 0.6624118858 2.9535015541 0.1952064601
C 2.8391246622 -0.2334899136 -2.2772036189
C 0.8327625565 3.6909417845 1.5300348762
C -0.2943750229 3.6858405377 -0.7488947917
C 3.7328211031 -0.1744061353 -1.0406870778
C 3.543208989 0.2580656041 -3.5450941367
C 0.3545505358 -2.7650417738 -7.1800867368
N 0.3945996794 -2.8664046429 -8.3383539098
H -0.995046085 -0.6343409591 -3.3318165792
H -0.927706408 -0.8674828724 -5.7932322616
H 1.5150831922 -4.3911432935 -5.3935083384
H 1.4400013249 -4.1519251769 -2.921541004
H 1.637057156 2.8234491537 -0.2813814213
H 2.4808649161 -1.2513425642 -2.4390499553
H 1.5559549804 3.1901378405 2.1804269804
H -0.1173699945 3.7708496698 2.0706522364
H 1.1906801251 4.7085918708 1.336074325
H -1.2895384713 3.7822763295 -0.3013654872
H -0.3986883635 3.1699639971 -1.7076993581
H 0.0883213157 4.6942029057 -0.9501010675
H 3.205277899 -0.5031260883 -0.1404476415
H 4.1092508255 0.8405030709 -0.8726030213
H 4.5946279957 -0.8381009623 -1.1847601722
H 3.8650507242 1.3009979302 -3.4460088633
H 2.899396002 0.1734078096 -4.4259123152
H 4.436436933 -0.3528335535 -3.7179065554

20_rot_ts:
E_{tot}=-1714.8861961 (-149.5 cm^{-1})

N -0.1305438287 -3.4194627569 -0.4533170026
C 0.2437238231 -2.311897323 -1.0578754782
O -0.2211191183 -3.1403437421 0.9070664221
C 0.4028096206 -2.3337166783 -2.525247864
C 0.9777946279 -1.2688107882 -3.2356129661
C 1.1194560066 -1.3207135852 -4.6185962447
C 0.4139116069 -1.2408328641 -0.1191030965
C 0.685935062 -2.4513840913 -5.3266222177
C 0.7194258657 0.1484929701 -0.2620593406
C 0.1095030063 -3.5263148627 -4.6244510396
C -0.0299109614 -3.4637940265 -3.2463981786
C 0.0961285352 -1.8047312531 1.1729832888
O 0.0987899302 -1.3538036195 2.306280092
S 2.3057984717 0.8366770159 -0.1646435301
S -0.6518736472 1.1517543653 -0.4375428869
C -0.1201116713 2.9462484376 -0.4271769077
C 3.414935743 -0.6151230599 0.2259696607
C 0.0841173922 3.4429658895 1.006663971
C -1.2091568558 3.72223339 -1.17604565
C 3.5209009742 -0.7895407599 1.7426424546
C 4.760603951 -0.3601254276 -0.4580804875
C 0.8293095052 -2.5067940748 -6.751042829
N 0.9475665917 -2.5474789811 -7.9080515703
H 1.3281266176 -0.3874091162 -2.7103684506
H 1.5666406383 -0.4900822009 -5.1553311133
H -0.2287377281 -4.4018856389 -5.1692618345
H -0.4769025699 -4.2875967345 -2.7016933904
H 0.8171598094 2.9977604223 -0.991150675
H 2.9121852754 -1.4766284479 -0.2203781759
H 0.8442095767 2.865379742 1.5395364752
H -0.8494774244 3.388669762 1.5759013798
H 0.4083150378 4.4903465608 0.9825069544
H -2.1804031971 3.6299112503 -0.6768360253
H -1.3176509095 3.3799030762 -2.2097201751
H -0.9447747 4.7854780704 -1.1939752421
H 2.5414903931 -0.9538502233 2.2001175612
H 3.989972114 0.0840918265 2.209399027
H 4.1511129642 -1.6626425369 1.9516043234
H 5.2455880845 0.5462401776 -0.0781143288
H 4.6598612772 -0.2733830253 -1.5442017628
H 5.4254321099 -1.2044701383 -0.2444341463

21:
E_{tot}=-1588.1908046

N 0.9403975679 -3.6638780591 -0.5967760625
C 1.447639603 -2.5255211124 -0.9645649312

O 0.436569132 -3.5430953832 0.7228469633
C 1.9870341757 -2.3445422282 -2.3645768961
C 1.7665641641 -3.4608519505 -3.4245262927
C 0.2671747279 -3.735256725 -3.6525841064
C 1.3032952988 -1.52267317 0.0921922323
C 1.6649844518 -0.1999154331 0.2085791644
C 0.5931203391 -2.2512404928 1.1617239953
O 0.2036253157 -1.8856913166 2.2494747033
S 2.7705277191 0.5736398778 -0.9718086775
S 1.0596469668 0.7275188886 1.5852164458
C 1.6118247054 2.4811801897 1.3138312278
C 4.3890969572 -0.2917316019 -0.5877081356
C 1.5483875401 3.1491379633 2.6938374293
C 0.7350036328 3.2002657941 0.2863104989
C 4.9190600356 0.0754158701 0.7968002567
C 5.3554013843 0.0948173363 -1.7101129484
C 2.3750013003 -2.9289539249 -4.7402192176
C 2.496284451 -4.763276774 -3.0397949769
H 3.0662975271 -2.154126853 -2.2977077714
H 1.5595245705 -1.4108663406 -2.7501670241
H -0.2658439517 -2.8139114632 -3.9208570873
H -0.2042271726 -4.1574480177 -2.7622507604
H 0.1353881447 -4.4453620895 -4.4780390974
H 2.6469934781 2.4507617667 0.9667567128
H 4.1847174068 -1.3649334571 -0.6314896564
H 2.2124667101 2.6596293491 3.4126783507
H 0.5312084498 3.1344985285 3.1018190027
H 1.854315687 4.1975981134 2.6015734884
H -0.3148623579 3.2009276383 0.5989525109
H 0.7982982516 2.7331260341 -0.7006786559
H 1.0629083045 4.242754179 0.1860026109
H 4.2091623438 -0.1861137264 1.5870211659
H 5.1361291429 1.1472219028 0.8637913516
H 5.8504988601 -0.4725648294 0.9883680959
H 5.5273205435 1.1771366727 -1.7310811104
H 4.9845989217 -0.2145847858 -2.6923667207
H 6.3220898165 -0.393136161 -1.5404856598
H 3.4465786372 -2.7175506027 -4.6305593461
H 1.8814990601 -2.00520632 -5.0676743405
H 2.2631160372 -3.6688285535 -5.5412376887
H 2.0818637503 -5.202448466 -2.1300155206
H 3.5669445663 -4.5809348146 -2.8777593357
H 2.4069398039 -5.4988974518 -3.8485881866

21_rot_ts:
E_{tot}=-1588.1570973 (-175.9 cm^{-1})

N -1.8232205332 -1.8321837965 -1.1640829538
C -0.6369248688 -1.3952928938 -1.5043252508
O -2.0716824238 -1.3765873589 0.1448000117

C -0.0042253967 -1.7272612097 -2.8365187892
C -0.8856162335 -1.6058327004 -4.1135567512
C -1.5476605868 -0.2174452743 -4.1834865685
C -0.032197624 -0.6455450271 -0.4417251887
C 1.2583354211 -0.0498235451 -0.3562537799
C -0.9929087413 -0.6484869741 0.6381266229
O -1.0059008431 -0.1425885417 1.7502726772
S 1.6390040618 1.5840335305 -0.7923080099
S 2.4737715095 -1.0762241084 0.276693987
C 4.069872623 -0.1160428909 0.4657843144
C -0.0150131594 2.3441609156 -1.2031110316
C 5.203390786 -1.1466245374 0.4246772708
C 4.0590410242 0.7024980689 1.7594292897
C 0.2258662451 3.4041425937 -2.2813609232
C -0.6630363096 2.8993531737 0.0670608087
C 0.04422655 -1.7854303006 -5.3305317599
C -1.9682333525 -2.7020650211 -4.14561148
H 0.3925095056 -2.7512958975 -2.7881545847
H 0.8697664167 -1.0739828368 -2.9608288001
H -0.7947201686 0.5829923271 -4.172002843
H -2.2306430356 -0.0637242067 -3.3420232377
H -2.1247727657 -0.1112373673 -5.1099865715
H 4.1447927731 0.5418846489 -0.4062415361
H -0.6089262411 1.5176677675 -1.6005901541
H 5.2213959312 -1.6960408081 -0.5215590148
H 5.1153148796 -1.8702666202 1.2431669707
H 6.1638693997 -0.631438204 0.5393038094
H 3.9812366594 0.0489396343 2.6343659306
H 3.2293964979 1.4139046022 1.7880476119
H 4.9952261847 1.268465023 1.8386148012
H 0.6610461776 2.9753118546 -3.1894147111
H 0.8825559985 4.2061555983 -1.9251217882
H -0.7357760666 3.8575727366 -2.5464162064
H -0.0532727069 3.6971092083 0.5066924527
H -0.8208504565 2.1168010514 0.8144338043
H -1.6388934979 3.3264358497 -0.1952345117
H 0.5576717843 -2.7546361268 -5.2994991557
H 0.810290977 -1.0002055201 -5.3720561834
H -0.5279510547 -1.7431993568 -6.2650253227
H -2.6370599481 -2.6217564723 -3.2856828283
H -1.5130898627 -3.7005947938 -4.1269432238
H -2.5618995288 -2.6238211942 -5.0652602035

Table S1. Natural population analysis charges and natural electron configurations for **12** – **19.**

| Compd | NPA charges | | | | | | difference | isoxazolone | twisting | hybridization | |
	C4	C6	C3	C5	X1	X2	C4-C6	fragm. charge	(°)	C4	C6
12	-0.307	-0.292	0.204	0.783	0.364	0.433	-0.015	-0.451	22	s0.89 p3.39	s1.04 p3.23
13	-0.308	-0.290	0.208	0.782	0.381	0.355	-0.018	-0.457	32	s0.90 p3.39	s1.04 p3.23
14	-0.360	0.148	0.205	0.768	0.335	-0.556	-0.508	-0.607	39	s0.89 p3.45	s0.90 p2.93
15	-0.381	0.519	0.195	0.760	-0.427	-0.410	-0.900	-0.702	40	s0.89 p3.48	s0.76 p2.69
16	-0.381	0.516	0.192	0.766	-0.407	-0.592	-0.897	-0.681	37	s0.89 p3.48	s0.77 p2.69
17	-0.395	0.535	0.190	0.751	-0.408	-0.400	-0.930	-0.757	45	s0.88 p3.50	s0.77 p2.67
18	-0.408	0.560	0.183	0.741	-0.600	-0.575	-0.968	-0.824	66	s0.89 p3.51	s0.78 p2.64
19(min1)	-0.403	0.566	0.185	0.736	-0.411	-0.407	-0.969	-0.823	66	s0.88 p3.51	s0.77 p2.64
19(min2)	-0.447	0.597	0.162	0.732	-0.403	-0.403	-1.044	-0.816	90	s0.87 p3.56	s0.78 p2.60