Additional comments to Table S1 and Figures S1-S4:

Since it is the mass of the anionic species identified experimentally, in most cases various products combinations (neutral species) are theoretically possible. The thresholds listed in Table S1 correspond to the combination of products (Fig. S1), where ΔG value was the lowest (for 0 eV experimental onset) or of the lowest deviation from experimental data.

Most of the fragment anions, except NO_2^- (mass 46 u) and (Metro-C_2H_4OH)$^-$ (126 u), form after multiple bond breakage. One may also expect that the OH^- anion arises from the single bond cleavage, but that would produce a threshold of 1.16 eV. Therefore, we suggest a bit more complicated neutral products (similar to these of (NO_2+C_2H_3OH)$^-$ (90 u)) that result in an exothermic threshold of –0.74 eV.

(Ring+H)$^-$ (66 u), (Ring+CH_3+H)$^-$ (81 u) and (NO_2+C_2H_3OH)$^-$ (90 u) anions require a bit more discussion as these are somehow connected. All three involve the product of 90 u mass, either as a radical or as an anion, arising from the recombination of NO_2 and C_2H_4OH with one hydrogen abstracted. Interestingly, all three could involve different hydrogen abstractions (C6–H, C7–H and O8–H). For the (Ring+H)$^-$ (66 u), the abstraction of the O8–H yields the ΔG value of 2.76 eV (best corresponding to the experimental value of 2.69 eV), while C6–H or C7–H would give 2.35 and 2.18 eV respectively. For (Ring+CH_3+H)$^-$ (81 u) abstraction of C7–H produces the lowest ΔG value of –0.86 eV, two other positions being 0.17 eV (C6–H) and 0.58 eV (O8–H) higher. It is worth noting, that in this case all three values are negative, therefore equally corresponding to the experimentally observed 0 eV. Finally, for (NO_2+C_2H_3OH)$^-$ (90 u) the fragment is in the anionic state and C7–H abstraction makes the molecule unstable, while other two are connected with the calculated threshold of –1.09 eV (C6–H) or –0.35 eV (O8–H) – again both positions are possible, as the experiment gives us the 0 eV threshold.

For (Metro-NO_2-OH)$^-$ (108 u) and (Metro-NO_2-CH_3)$^-$ (110 u) two bonds break, initially producing two radicals (NO_2 and OH or CH_3). It is worth noting, that (probably due to the distance between these) for the first case NO_2 and OH combine to give $HONO_2$ molecule. If that is not the case we would not observe the threshold of 1.99 eV, but instead 2.90 eV. Similarly, from the fact that we observe the threshold of 2.77 eV and not 1.44 eV, we can conclude that NO_2 does not combine with CH_3 in case of (Metro-NO_2-CH_3)$^-$ (110 u).

While from the remaining, (Metro-CHOH-NO_2)$^-$ (95 u) and (Metro-NO_2-2H)$^-$ (123 u) are pretty straightforward, (NO_2+N+C_2H_4OH)$^-$ (105 u), CN^- (26 u) and CNO^- (42 u) formation involve more complicated mechanisms, including bond cleavage in the ring and further rearrangements, see Figure S2-S4. These are difficult to assess having only anion masses. For the first one, (NO_2+N+C_2H_4OH)$^-$ (105 u), depending on the rearrangements that could occur after the initial bond breaks we've found the thresholds energies ranging from –0.53 eV to even 3.85 eV. The most probable value of 1.20 eV (0.76 eV lower than the experimental value) also seems to be one of the least complicated. Similarly, for the CN^- anion (26 u) we've found 0.74 eV (1.86 eV lower than the experimental value) that corresponds to pretty simple fragmentation scheme. The calculated CNO^- (42 u) anion threshold is 0.78 eV lower than the experimental one and thus a possible scheme to explain the experimental result.

Table S1. The calculated thresholds and AEA of anions, as calculated at M06-2X/aug-cc-pvtz level of theory. All values shown in eV.

Mass (u)	Reaction anionic product	M06-2X/aug-cc-pvtz					Experimental
			1 atm		*2.92x10^{-11} atm*		
		AEA	298.15 K	360.15 K	298.15 K	360.15 K	
17	OH^-	1.66	2.03	1.52	0.16	**-0.74**	**0**
26	CN^-	4.07	2.50	2.25	1.25	**0.74**	**2.60**
42	CNO^-	3.41	2.64	2.53	2.01	**1.78**	**2.56**
46	NO_2^-	2.35	0.53	0.40	-0.10	**-0.35**	**0**
66	$(Ring+H)^-$	3.02	4.52	4.27	3.27	**2.76**	**2.69**
81	$(Ring+CH_3+H)^-$	2.40	0.03	-0.11	-0.60	**-0.86**	**0**
90	$(NO_2+C_2H_3OH)^-$	2.83	-0.21	-0.34	-0.84	**-1.09**	**0**
95	$(Metro\text{-}CHOH\text{-}NO_2)^-$	1.83	1.37	1.13	0.12	**-0.38**	**0**
105	$(NO_2+N+C_2H_4OH)^-$	3.44	2.08	1.96	1.45	**1.20**	**1.96**
108	$(Metro\text{-}NO_2\text{-}OH)^-$	1.96	2.88	2.74	2.25	**1.99**	**2.15**
110	$(Metro\text{-}NO_2\text{-}CH_3)^-$	3.11	4.52	4.28	3.27	**2.77**	**2.63**
123	$(Metro\text{-}NO_2\text{-}2H)^-$	2.26	-0.39	-0.59	-1.64	**-2.09**	**0**
126	$(Metro\text{-}C_2H_4OH)^-$	3.64	-0.58	-0.72	-1.21	**-1.47**	**0**
171	$Metro^-$	1.24					**0**

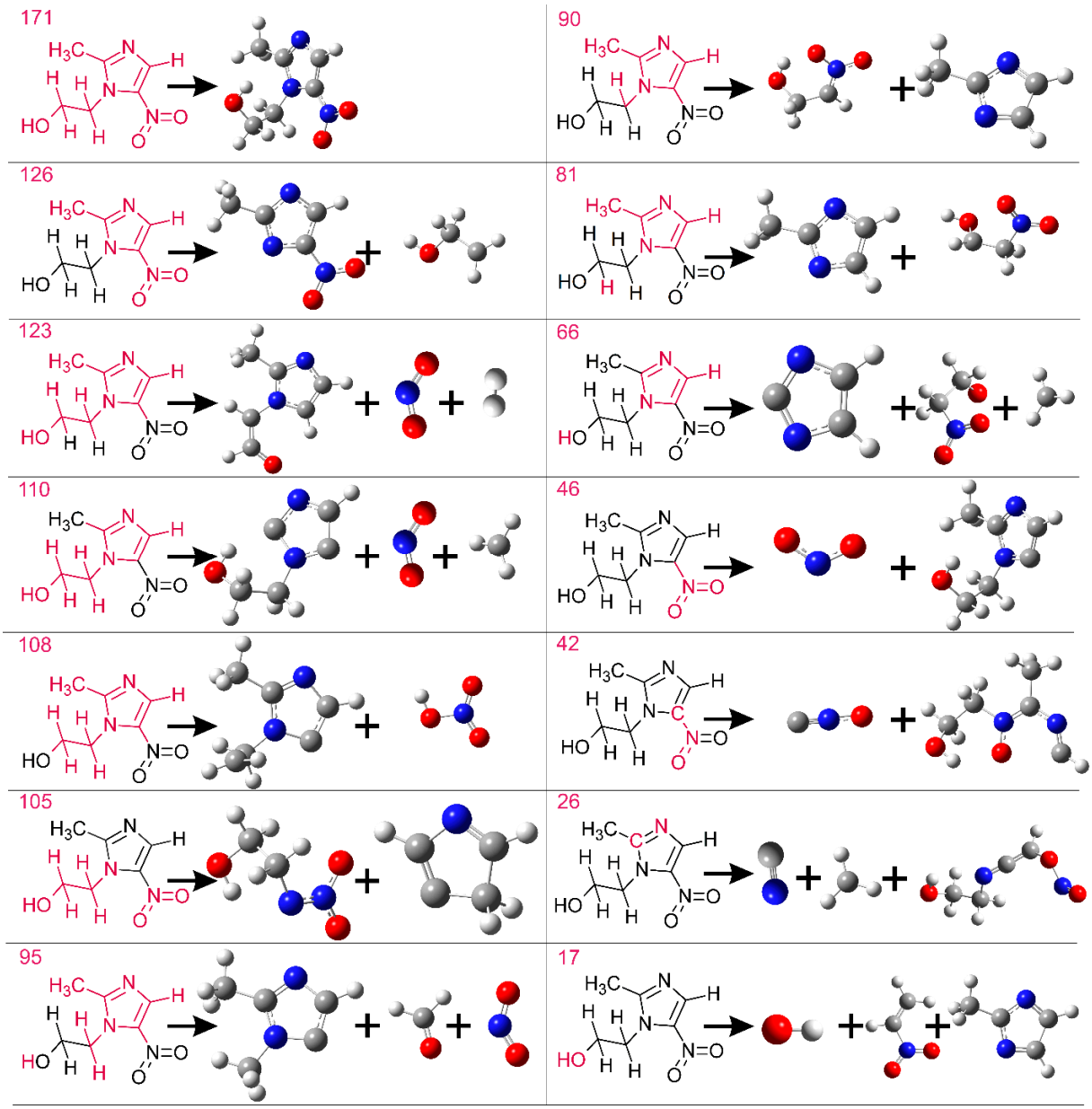

Figure S1. Possible dissociation pathways for the observed anions upon electron attachment to Metro.

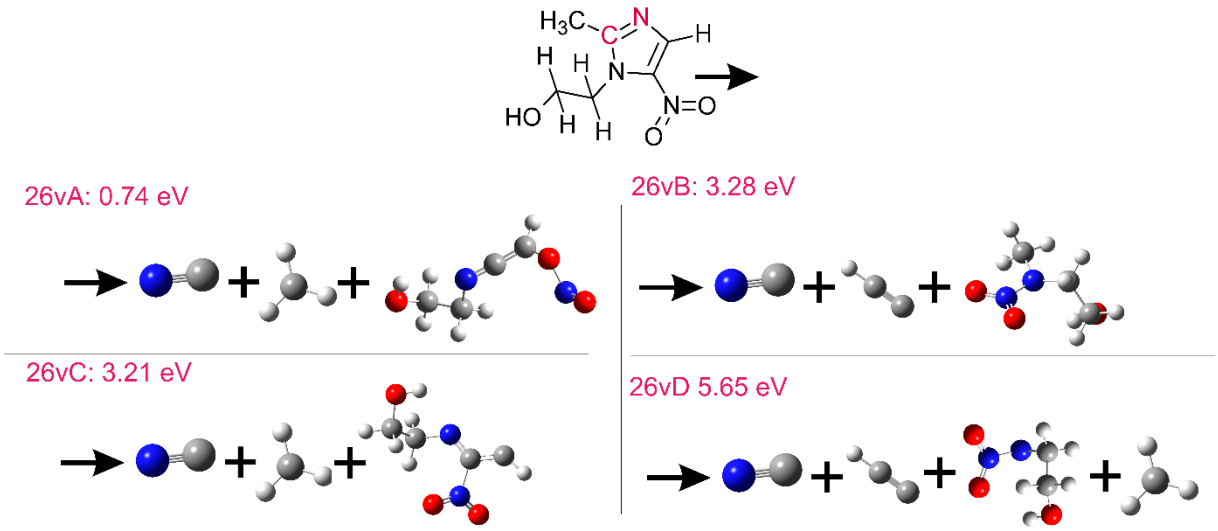

Figure S2. Possible dissociation pathways leading to CN^- upon electron attachment to Metro.

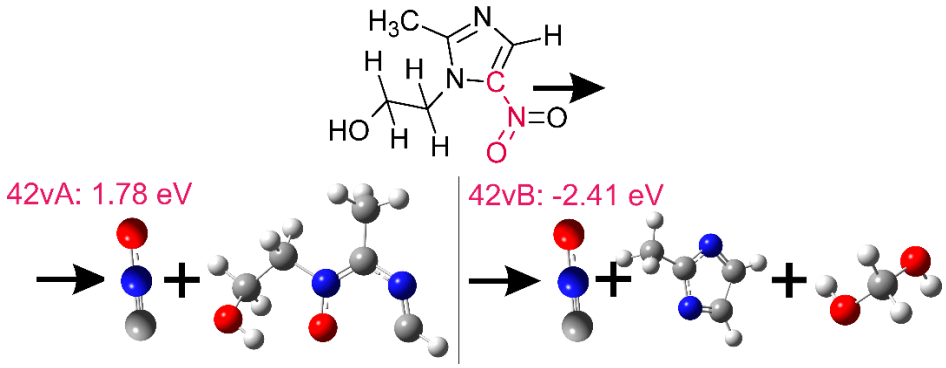

Figure S3. Possible dissociation pathways leading to CNO^- upon electron attachment to Metro.

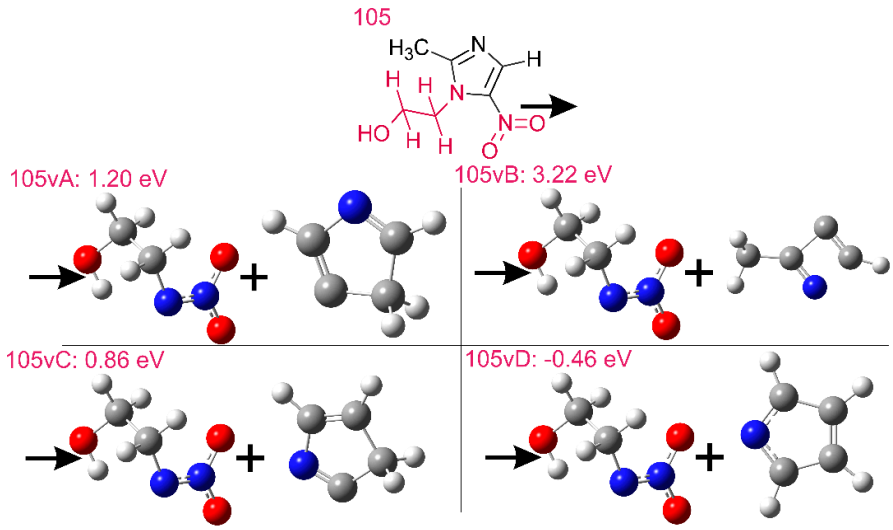

Figure S4. Possible dissociation pathways leading to $(NO_2+N+C_2H_4OH)^-$ upon electron attachment to Metro.

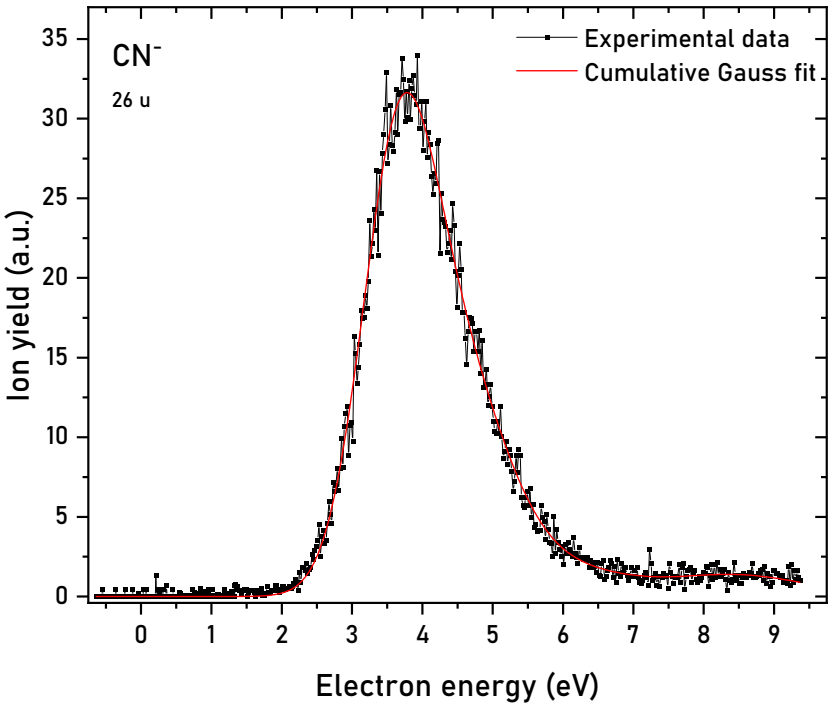

Figure S5. Anion efficiency curve for CN^- formed upon electron attachment to isolated Metro.

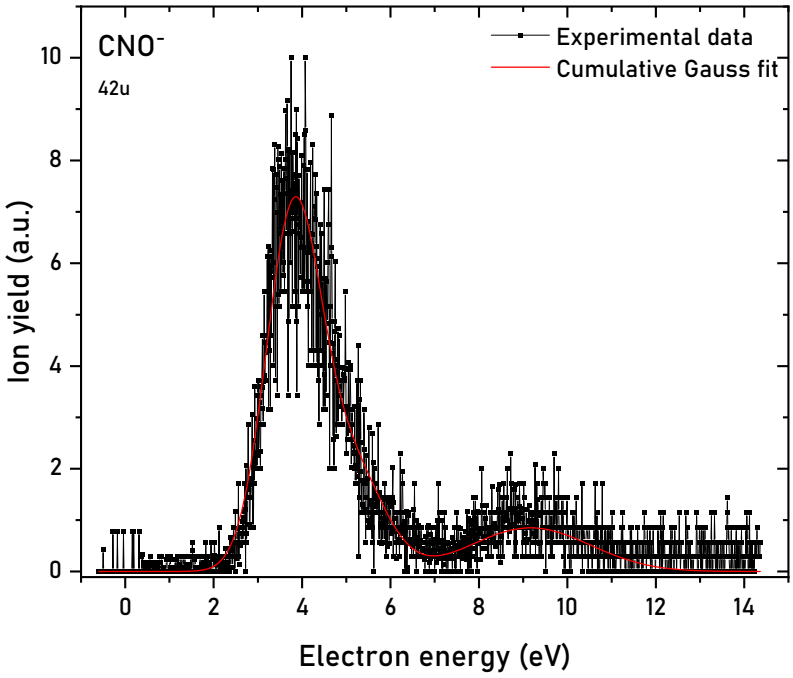

Figure S6. Anion efficiency curve for CNO^- formed upon electron attachment to isolated Metro.

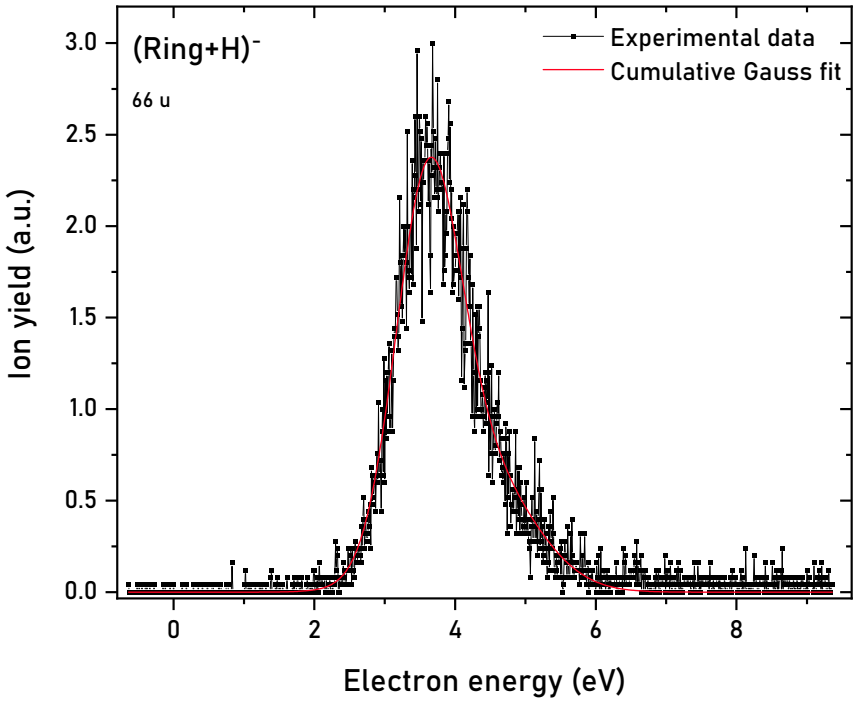

Figure S7. Anion efficiency curve for $(Ring+H)^-$ formed upon electron attachment to isolated Metro.

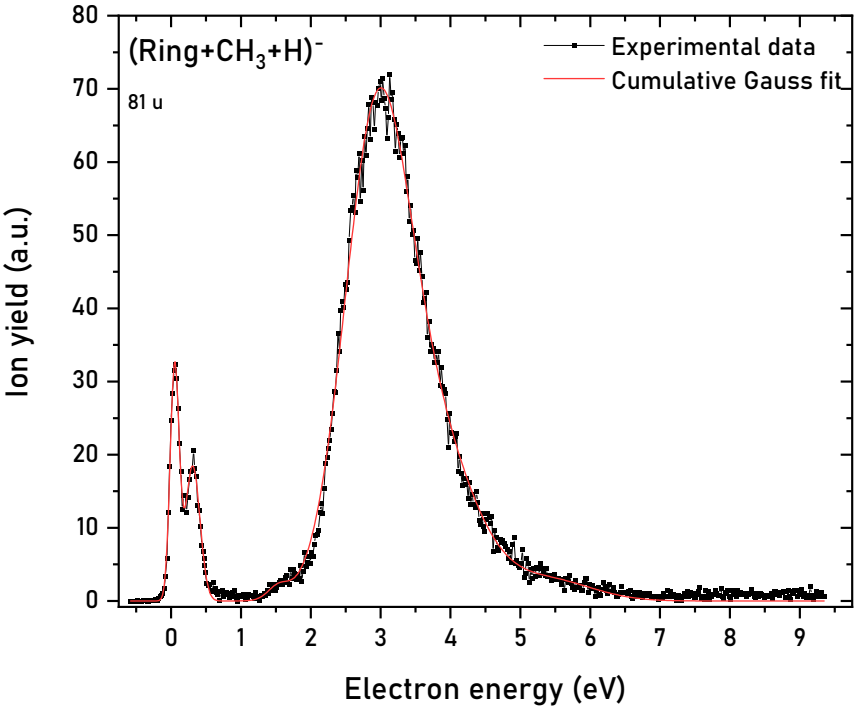

Figure S8. Anion efficiency curve for $(Ring+CH_3+H)^-$ upon electron attachment to isolated Metro.

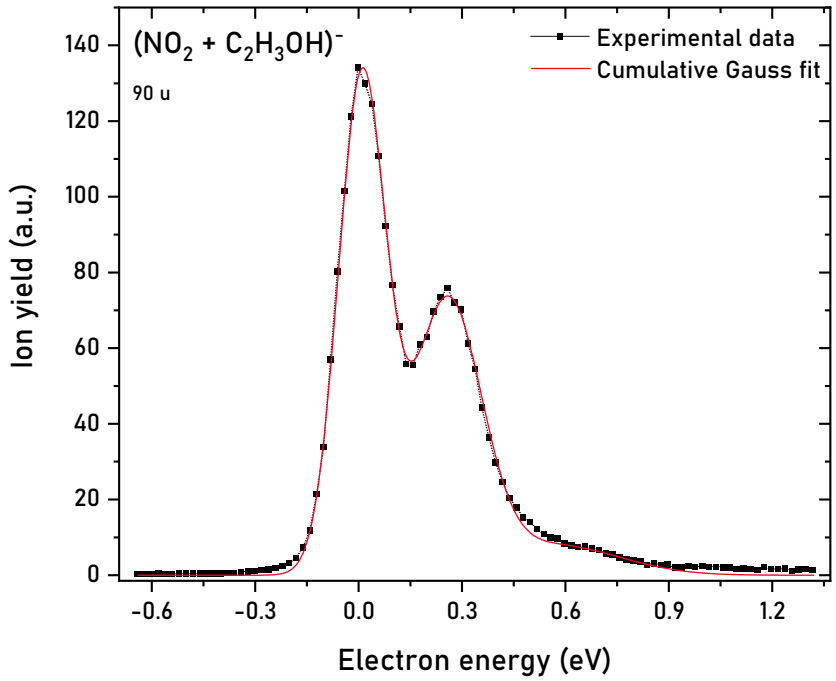

Figure S9. Anion efficiency curve for $(NO_2+C_2H_3OH)^-$ formed upon electron attachment to isolated Metro.

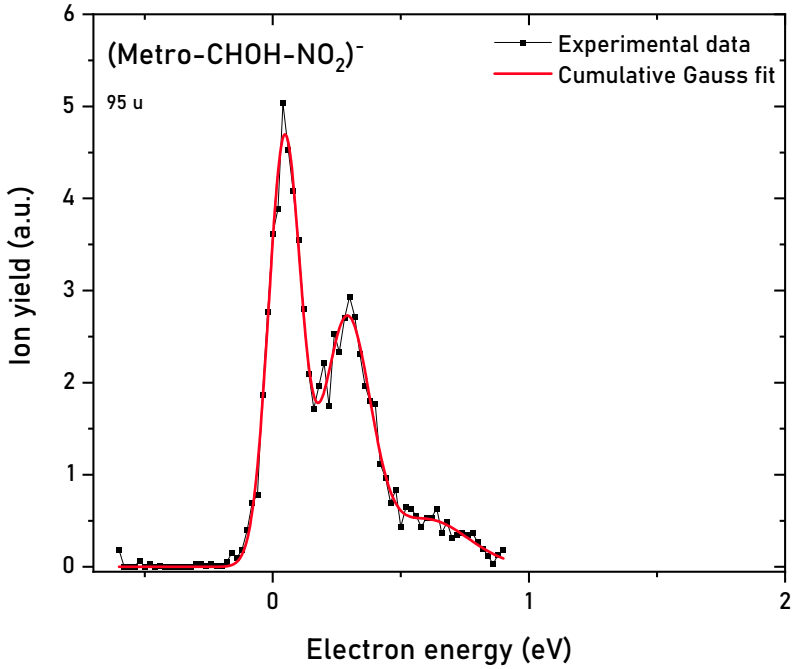

Figure S10. Anion efficiency curve for $(Metro\text{-}CHOH\text{-}NO_2)^-$ formed upon electron attachment to isolated Metro.

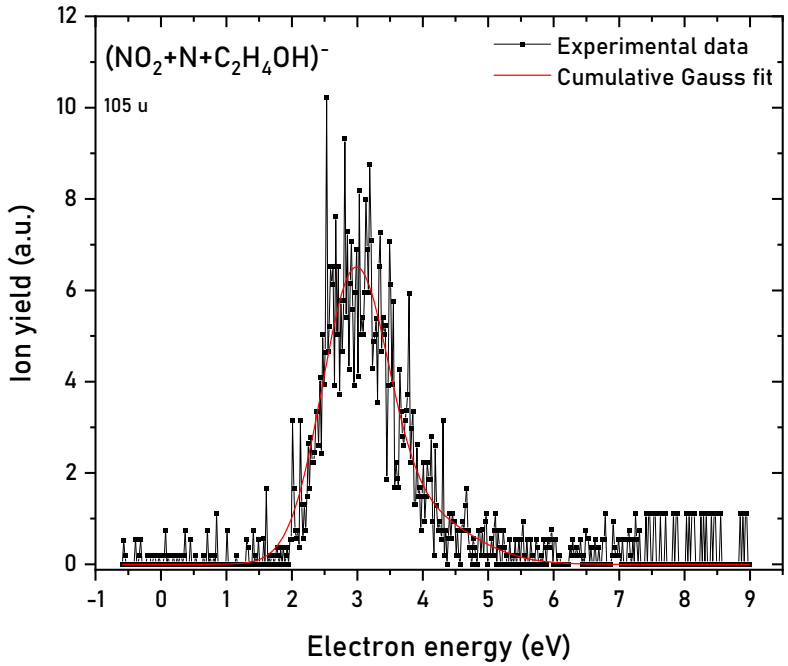

Figure S11. Anion efficiency curve for $(NO_2+N+C_2H_4OH)^-$ formed upon electron attachment to isolated Metro.

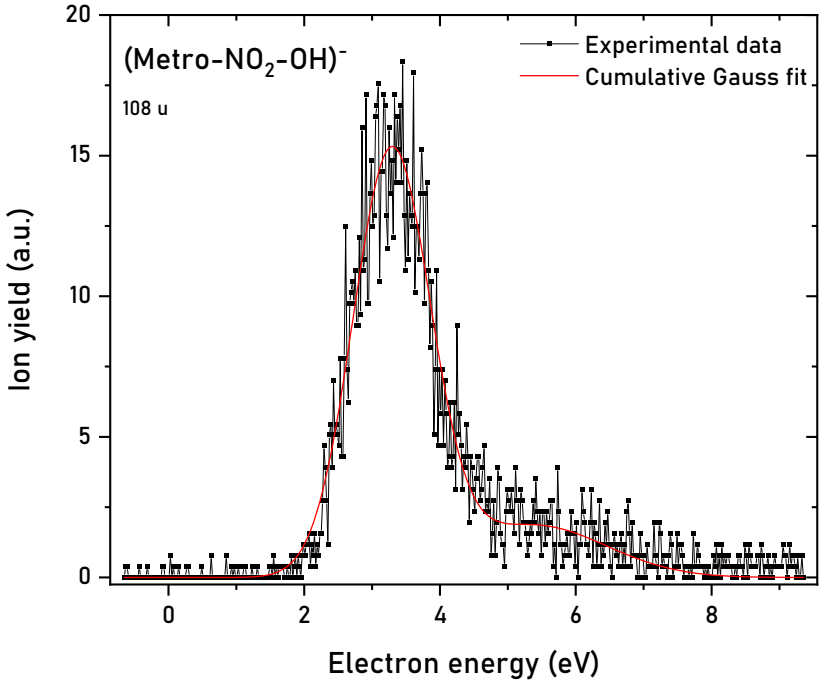

Figure S12. Anion efficiency curve for $(Metro\text{-}NO_2\text{-}OH)^-$ formed upon electron attachment to isolated Metro.

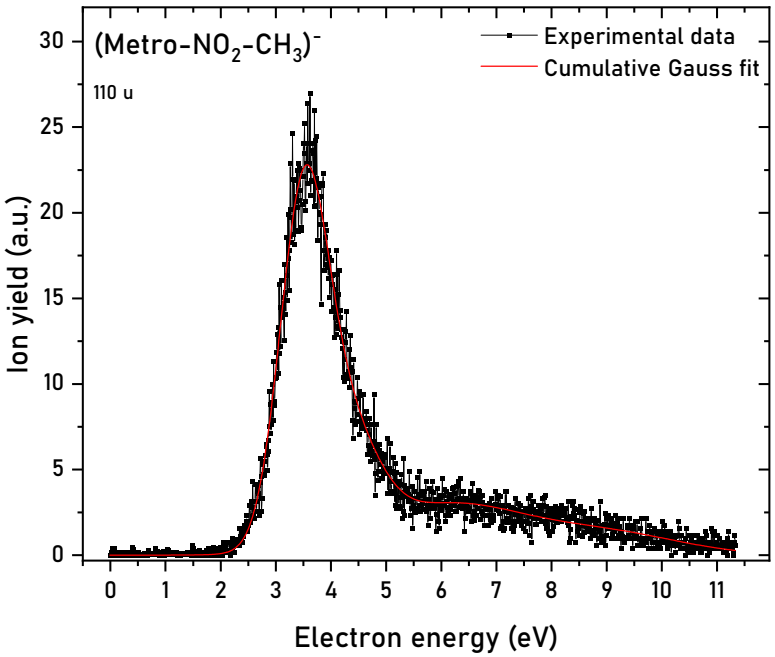

Figure S13. Anion efficiency curve for $(Metro\text{-}NO_2\text{-}CH_3)^-$ formed upon electron attachment to isolated Metro.

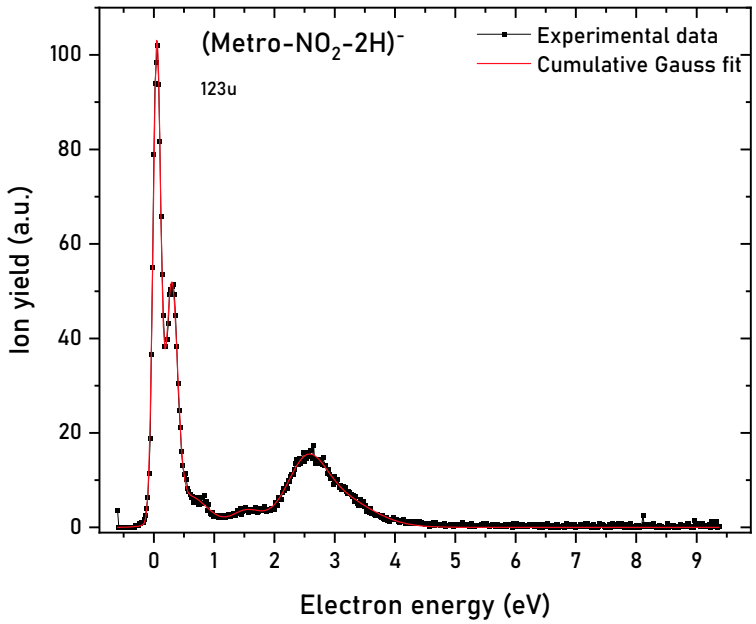

Figure S14. Anion efficiency curve for $(Metro\text{-}NO_2\text{-}2H)^-$ formed upon electron attachment to isolated Metro.

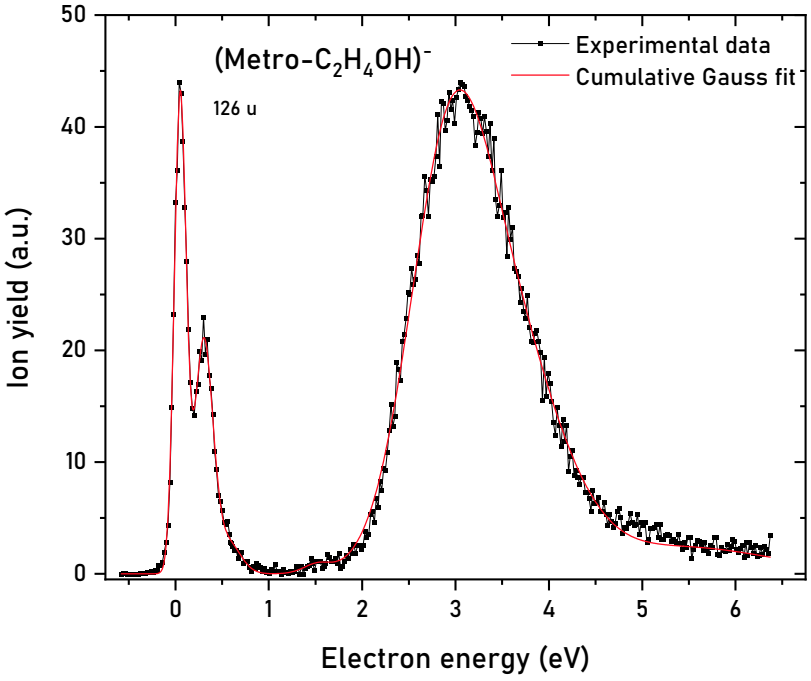

Figure S15. Anion efficiency curve for $(Metro\text{-}C_2H_4OH)^-$ formed upon electron attachment to isolated Metro.

XYZ coordinates for the structures shown in Figure S1-S4

SUBSTRATE:

METRONIDAZOLE - NEUTRAL

N	1.474617	5.087138	7.241081
C	1.017146	6.174539	6.573189
C	0.940537	7.535616	7.166151
H	1.923844	7.897432	7.468936
H	0.283632	7.542789	8.034864
H	0.540675	8.203825	6.409844
N	0.651948	5.884420	5.335095
C	0.867212	4.559560	5.180601
H	0.663993	4.026500	4.268310
C	1.369995	4.043513	6.343232
C	1.910771	5.063536	8.633641
H	2.799224	4.445849	8.715656
H	2.168448	6.087653	8.899282
C	0.819103	4.546756	9.558180
H	0.474865	3.576767	9.206061
H	1.238053	4.410872	10.557983
O	-0.304206	5.407068	9.576194
H	-0.166167	6.100704	10.224309
N	1.740076	2.696948	6.604969
O	1.612757	1.905746	5.695622
O	2.158315	2.415113	7.717867

PRODUCTS:

MASS 171

N	1.459824	5.086203	7.241265
C	1.000789	6.191327	6.566452
C	0.916984	7.547107	7.176695
H	1.888283	7.910164	7.523402
H	0.225777	7.572796	8.022644
H	0.549298	8.225602	6.411050
N	0.658764	5.907547	5.336797
C	0.883819	4.562426	5.177770
H	0.693132	4.032604	4.263420
C	1.377556	4.024757	6.348093
C	1.877960	5.051505	8.627919
H	2.761730	4.427019	8.710241
H	2.128534	6.075575	8.919693
C	0.811845	4.502374	9.559979
H	0.444665	3.563035	9.156015
H	1.267869	4.300627	10.535853
O	-0.306480	5.371720	9.703863
H	0.015178	6.228622	9.992198
N	1.735945	2.729292	6.631879
O	1.589487	1.864633	5.703384
O	2.203879	2.437409	7.802452

MASS 126

N	1.304146	5.057226	7.330210
C	1.057267	6.136954	6.602579
C	0.932249	7.500676	7.202265

H	1.675410	8.181339	6.782302
H	1.074925	7.440966	8.279219
H	-0.051037	7.928527	6.997197
N	0.921752	5.934021	5.261369
C	1.097438	4.613881	5.126014
H	1.056107	4.098902	4.180135
C	1.331026	4.078123	6.389629
N	1.565701	2.718852	6.689632
O	1.567821	1.914863	5.752817
O	1.757490	2.376991	7.847877
C	1.967695	5.131997	8.870562
H	2.972624	4.776369	9.036392
H	1.784044	5.821266	8.059590
C	0.815526	4.511313	9.564954
H	0.391172	3.694061	8.971273
H	1.134785	4.073844	10.517029
O	-0.258596	5.418396	9.759119
H	0.087294	6.203778	10.190901

MASS 123

c	0.217052	0.021456	-0.116963
n	-0.060874	-0.045888	1.226079
c	1.139419	0.013379	1.862324
n	2.149284	0.117165	1.019442
c	1.574392	0.116411	-0.226921
c	-1.356604	-0.182285	1.829346
c	-1.934035	0.888362	2.476123
o	-3.027635	0.949153	3.084322
c	1.260530	-0.039817	3.344967
h	0.702167	-0.886332	3.744815
h	0.847017	0.855745	3.809315
h	2.313396	-0.128168	3.602621
h	2.169091	0.189014	-1.123136
h	-1.814539	-1.159416	1.768763
h	-1.302245	1.808896	2.426153
h	-0.579064	0.006535	-0.839505
n	0.073919	-0.000000	0.047505
o	-0.058869	0.000000	1.220393
o	0.997313	0.000000	-0.687135
H	0.000000	0.000000	0.233779
H	0.000000	0.000000	0.972811

MASS 110

N	1.448564	5.021613	7.306127
C	0.297511	5.800629	7.025758
N	0.080196	5.654608	5.677673
C	0.968662	4.767186	5.244923
H	0.979151	4.445915	4.209310
C	1.877540	4.258660	6.268897
C	1.958451	4.929423	8.661409
H	2.693016	4.124987	8.674022
H	2.453349	5.867097	8.931651
C	0.851383	4.661081	9.671933
H	0.335644	3.736187	9.378958
H	1.299707	4.496953	10.656225

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 O    -0.050135    5.733894    9.783089
 H    -0.238184    5.998411    8.839015

 n     0.073919   -0.000000    0.047505
 o    -0.058869    0.000000    1.220393
 o     0.997313    0.000000   -0.687135

 c     0.384284    0.221866    0.093648
 h    -0.083260   -0.048070    1.025046
 h     1.086073   -0.449663   -0.370722
```

MASS 108

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 N     1.591202    5.024050    7.155372
 C     0.974854    6.117930    6.607882
 C     0.803246    7.416467    7.324889
 H     1.763475    7.872082    7.590271
 H     0.233843    7.304514    8.252801
 H     0.270403    8.102374    6.669371
 N     0.591770    5.863320    5.382723
 C     0.984461    4.544834    5.175575
 H     0.779722    4.084906    4.218556
 C     1.621437    3.947964    6.256409
 C     2.065144    4.956535    8.513508
 H     2.740600    4.094098    8.544863
 H     2.662951    5.843218    8.758955
 C     0.965545    4.799134    9.504977
 H     0.081020    4.253810    9.211109
 H     1.117852    5.034720   10.549647

 H     1.023434    3.914917    5.174988
 N     1.665335    2.708326    6.441370
 O     1.628703    1.902831    5.551180
 O     1.998113    2.577554    7.571551
 O     1.257586    3.984513    6.113544
```

MASS 105

vA-vD

```
 h     0.392020    0.108765   -0.134252
 o     0.171061    0.237442    0.799281
 h     1.153680   -0.249997    2.512583
 c     1.399104    0.004006    1.478068
 h     2.017655    0.905309    1.472007
 h     1.573131   -2.044365    0.901288
 h     3.129133   -1.268004    1.299988
 c     2.164907   -1.129874    0.804230
 n     2.293930   -0.890490   -0.621018
 o     4.055538    0.365632   -0.036158
 o     3.470590    0.183971   -2.118022
 n     3.286114   -0.101327   -0.917839
```

vA

```
 c    -0.046010   -0.059778    0.022327
 c     0.027216   -0.046855    1.506426
 c     1.286324    0.008923    1.913487
 n     2.163773    0.038519    0.777384
 c     1.428793   -0.000908   -0.269620
 h    -0.507195   -0.963634   -0.381896
 h    -0.580652    0.796768   -0.394232
```

```
 h     1.701307    0.033369    2.906651
 h     1.858619    0.010601   -1.263658

vB
 C     0.658473   1.062549  -0.00009000
 C     1.602914  -0.012487   0.00024000
 N     0.563829  -0.920209  -0.00011700
 C    -0.388881   0.085510  -0.00020900
 C    -1.855836  -0.012167   0.00004900
 H    -2.147791  -1.060007  -0.00762400
 H    -2.281582   0.480721  -0.87573400
 H    -2.280265   0.466968   0.88415300
 H     2.662813  -0.186643   0.00008700

vC
 C      0.417121   1.054904  -0.00017000
 C    -0.877647   0.732814   0.00008000
 N    -1.081376  -0.695550   0.00003500
 C     0.055367  -1.199161  -0.00024200
 C     1.204800  -0.228242   0.00008200
 H     1.836083  -0.359248  -0.88020500
 H     1.834550  -0.359173   0.88155600
 H    -1.740220   1.379567   0.00017200
 H     0.841368   2.045810  -0.00027000

vD
 C     0.979574  -0.676365   0.00009500
 C    -0.422984  -1.058706  -0.00008200
 N    -1.239892  -0.000607   0.00003100
 C    -0.424133   1.058238   0.00006500
 C     0.978921   0.677349  -0.00005600
 H     1.820683   1.349296  -0.00018600
 H    -0.814836  -2.065540  -0.00012600
 H     1.822182  -1.347302   0.00007700
 H    -0.817056   2.064702  -0.00011200

MASS 95

 c    -0.145548   -0.088311    0.028418
 n     0.018408   -0.061631    1.421054
 c     1.341257   -0.016588    1.765801
 n     2.099294   -0.010541    0.698346
 c     1.190381   -0.054364   -0.353513
 c    -1.059325   -0.079009    2.371622
 c     1.818303    0.020116    3.179321
 h     1.500128   -0.860412    3.747678
 h     1.447942    0.898014    3.719548
 h     2.905970    0.052356    3.176544
 h     1.566561   -0.059017   -1.367435
 h    -1.008650   -0.952937    3.030364
 h    -1.061757    0.816683    3.002533
 h    -1.986219   -0.115756    1.805141

 C     0.320046    0.395640    0.358346
 H     1.159727   -0.176798   -0.072776
 H    -0.097397    1.204027   -0.264968
 O    -0.115010    0.151425    1.445262

 N     0.073919   -0.000000    0.047505
 O    -0.058869    0.000000    1.220393
```

```
 O     0.997313    0.000000   -0.687135
```

MASS 90

```
 c    -0.037935    0.376819    0.068341
 c     0.092464   -0.174123    1.442680
 o     1.173778    0.382430    2.190391
 n     1.001997    0.303644   -0.747229
 o     2.096081   -0.210025   -0.303519
 o     0.954649    0.734054   -1.935924
 h    -0.914481    0.865015   -0.319236
 h     0.227552   -1.265038    1.408490
 h     1.908926    0.302202    1.557894
 h    -0.822269    0.032933    2.000870

 N     1.461534    5.096518    7.321949
 C     0.989587    6.179598    6.619034
 N     0.617473    5.914203    5.332529
 C     0.855109    4.629808    5.201320
 H     0.668493    4.087002    4.287350
 C     1.387242    4.115956    6.460504
 H     1.685254    3.103958    6.691168
 C     0.899851    7.521952    7.223939
 H     0.273761    7.481702    8.116828
 H     1.890231    7.844134    7.550615
 H     0.492692    8.234539    6.513968
```

MASS 81

```
 N     1.453950    5.106222    7.318071
 C     0.996847    6.164384    6.631219
 N     0.629371    5.924102    5.363364
 C     0.872530    4.587748    5.220104
 H     0.677486    4.068757    4.291525
 C     1.373874    4.091447    6.409013
 H     1.673633    3.081369    6.653525
 C     0.904036    7.530882    7.240491
 H     0.266568    7.529760    8.128522
 H     1.885846    7.898684    7.550798
 H     0.487085    8.226015    6.512572

 C     1.068406    3.967206    6.445577
 N     1.972960    2.738755    6.520374
 O     2.582722    2.402759    5.541059
 O     2.022774    2.195398    7.609180
 C     1.540539    4.993270    7.383898
 H     1.092812    4.304243    5.416315
 H     1.879129    5.965238    7.071939
 O     1.539707    4.763240    8.707358
 H     1.516896    3.808624    8.868624
 H     0.085815    3.566121    6.710973
```

MASS 66

```
 N     1.470481    5.081848    7.333493
 C     1.014410    6.103516    6.634906
 N     0.632526    5.931035    5.384536
 C     0.872129    4.581118    5.223207
 H     0.668661    4.076223    4.288735
 C     1.378691    4.067877    6.401503
```

H	1.676352	3.054622	6.633487
c	0.026243	0.108899	-0.022013
n	0.039520	-0.018891	1.475858
o	1.061195	0.285718	2.046851
c	1.350954	-0.330140	-0.613751
o	1.609715	-1.660851	-0.455676
o	-0.981523	-0.384765	2.003367
h	-0.170681	1.162685	-0.215053
h	-0.804929	-0.497481	-0.366102
h	2.181728	0.208909	-0.134476
h	1.397949	-0.064519	-1.678315
c	0.384284	0.221866	0.093648
h	-0.083260	-0.048070	1.025046
h	1.086073	-0.449663	-0.370722
h	0.153617	1.165399	-0.370722

MASS 46

N	-0.042962	0.000000	-0.017495
O	0.013845	-0.000000	1.225248
O	1.041481	0.000000	-0.626990
N	1.484040	5.120341	7.251374
C	0.994726	6.200115	6.568885
C	0.876369	7.561015	7.156833
H	1.835787	7.928292	7.524991
H	0.161180	7.572858	7.979138
H	0.526133	8.230806	6.376466
N	0.654404	5.871673	5.346276
C	0.912313	4.524531	5.200806
H	0.725444	3.995473	4.285037
C	1.413433	4.077079	6.375967
C	1.917618	5.035204	8.629736
H	2.768836	4.354858	8.678376
H	2.258391	6.023027	8.942443
C	0.815214	4.541845	9.555082
H	0.405921	3.612524	9.159568
H	1.240560	4.333751	10.541209
O	-0.263967	5.448097	9.639155
H	-0.012830	6.190229	10.193910

MASS 42

vA-vB

c	-0.280757	0.000000	0.154199
n	0.420797	0.000000	1.091060
o	1.179893	0.000000	2.101407

vA

O	-0.444752	1.314015	1.063912
N	0.150199	0.612511	1.950314
C	1.640363	0.610914	1.918418
H	1.991006	1.181097	2.779778
H	1.982676	-0.419062	2.010354
C	2.155591	1.237955	0.638652
H	3.235715	1.092929	0.611831
H	1.718845	0.721628	-0.220048
H	0.954218	2.710324	0.571294

```
 O     1.916244    2.619271    0.587458
 C    -0.476914   -0.052800    2.882224
 C     0.259525   -0.864415    3.898942
 H     0.753748   -1.726207    3.447602
 H    -0.460410   -1.224224    4.627047
 H     1.018138   -0.278784    4.418855
 N    -1.850215    0.037550    2.996926
 C    -2.621836    0.507846    2.146416
 H    -3.694039    0.646350    2.302861

vB
 N    -0.153643   1.158119  -0.00381000
 C     0.587878   0.010631  -0.00737400
 N    -0.143707  -1.152783  -0.00392400
 C    -1.382968  -0.735830   0.00290500
 C    -1.392215   0.724778   0.00303300
 C     2.062842   0.004959   0.00108000
 H    -2.247050   1.384488   0.00711500
 H     2.419715  -0.372113   0.96269300
 H     2.435935  -0.678360  -0.76180700
 H     2.450419   1.006194  -0.15854300
 H    -2.230791  -1.404798   0.00681800

vB
 H     0.004119   1.157750   0.89231000
 O    -1.159848  -0.246877   0.09454900
 H    -1.237070  -0.775379  -0.70490200
 H    -0.004436   1.157238  -0.89287100
 C    -0.000014   0.530787  -0.00011800
 O     1.159681  -0.247011  -0.09456500
 H     1.238806  -0.773227   0.70630100
```

MASS 26

```
vA-vD
 c     0.0000   0.0000   0.136038
 n     0.0000   0.0000   1.303962

vA,vC,vD
 c     0.384284    0.221866    0.093648
 h    -0.083260   -0.048070    1.025046
 h     1.086073   -0.449663   -0.370722
 h     0.153617    1.165399   -0.370722

vA
 h    -0.715610   -0.023611   -0.199829
 h     0.728203   -0.049451    1.815444
 h     1.521132   -0.890108    0.457631
 c     0.681087   -0.915394    1.154760
 c    -0.651205   -0.911582    0.427824
 h    -0.716661   -1.792241   -0.219864
 o    -1.729941   -0.8607   1.329384
 h    -1.618442   -1.576394    1.963442
 n     0.736391   -2.105869    2.012678
 c     1.716998   -2.811702    2.091431
 c     2.738620   -3.629620    2.200125
 h     2.854474   -4.482282    1.549892
 o     3.719256   -3.431562    3.155585
 n     4.500528   -2.263494    2.870633
 o     5.288330   -2.096140    3.695512
```

vB,vD

C	0.476219	0.000045	0.000000
C	-0.745635	-0.000022	0.000000
H	1.616494	-0.000141	0.000000

vB

C	1.928259	-0.662487	0.06570900
C	0.836835	-0.104833	0.96236400
N	-0.287488	0.414598	0.18788000
N	-1.282715	-0.458487	-0.11268500
O	-1.039460	-1.6445	0.01888400
O	2.442935	0.334946	-0.79420000
O	-2.331518	0.009350	-0.51068300
H	1.8116	0.486227	-1.50170300
H	2.757533	-1.000887	0.68611200
H	1.545522	-1.517387	-0.49471000
H	1.232356	0.737686	1.52689700
H	0.482046	-0.866291	1.65595800
C	-0.641619	1.823433	0.19267700
H	-1.098597	2.093415	-0.75423900
H	-1.338578	2.061096	0.99886700
H	0.283028	2.378318	0.31994200

vC

H	2.785907	-1.526558	0.11213100
H	1.670590	-0.068035	1.77870100
H	0.544897	-1.229447	1.02965600
C	1.158942	-0.345448	0.85653600
C	2.221087	-0.649335	-0.19941300
H	1.724821	-0.876521	-1.14743100
O	3.144435	0.404908	-0.33510200
H	2.654333	1.217398	-0.49154000
N	0.413457	0.821126	0.43307300
C	-0.789073	0.804098	0.02204700
C	-1.531089	1.911516	-0.36384300
H	-2.538371	2.072737	-0.70336700
O	-2.703718	-0.497626	0.38228400
N	-1.593569	-0.503019	-0.09074300
O	-1.058292	-1.424946	-0.65548400

vD

H	-1.371095	-1.408198	0.41750800
O	-2.057161	-0.791746	0.14058700
H	-2.278141	0.749606	-1.14077200
C	-1.470445	0.204423	-0.65431100
H	-0.840169	-0.223951	-1.43990200
H	-1.301779	1.710312	0.90206200
H	-0.223963	1.961193	-0.49512000
C	-0.667135	1.212282	0.17373600
N	0.416523	0.613675	0.93563000
O	2.042760	0.374180	-0.56356300
O	0.956264	-1.368199	0.11421200
N	1.198581	-0.185543	0.08005200

MASS 17

O	0.00	0.00	0.122270
H	0.00	0.00	1.084321

C	1.249616	4.070187	6.452150
N	1.862376	2.740611	6.571838
O	1.633979	1.975526	5.660285
O	2.538917	2.494576	7.543435
C	1.440949	4.975031	7.386928
H	0.671528	4.162122	5.547997
H	2.049254	4.749048	8.250937
H	0.988103	5.950933	7.294867
N	1.471148	5.083147	7.300948
C	1.015521	6.164331	6.584160
C	0.947511	7.515859	7.171056
H	1.947843	7.838462	7.465666
H	0.346121	7.492072	8.081691
H	0.526060	8.220014	6.461481
N	0.641180	5.888284	5.300479
C	0.859447	4.598835	5.185839
H	0.665627	4.047306	4.278275
C	1.384209	4.093155	6.451481
H	1.6673	3.079851	6.695054