

Electronic Supporting Information

CHNO isomers and derivatives - A computational overview

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Estimation of RSE

As reported elsewhere,^{S1} RSEs were calculated using homodesmotic reactions (reaction class 4 or "RC4"), which constitute the penultimate type in a hierarchy of increasingly accurate processes, due to the conservation of larger fragments, according to a recent classification and redefinition of reaction types used in thermochemistry.^{S2} RSE were obtained as the average of the opposite energy (including the zero-point energy correction) for the three endocyclic bond cleavage reactions (Figure S1).

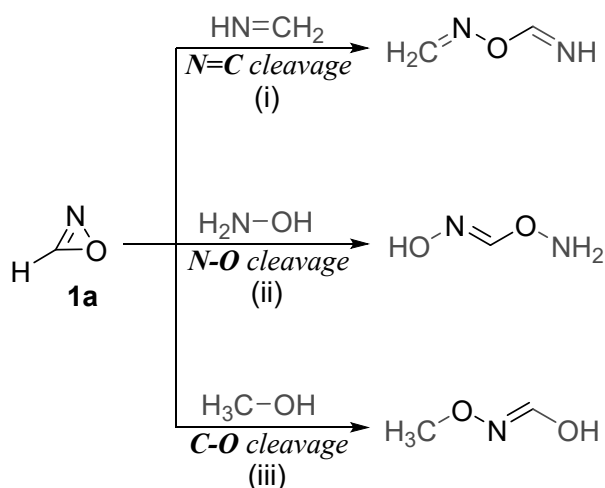


Figure S1: Homodesmotic (RC4)^{S2} ring-opening reactions used for the estimation of RSE of **1a**.

^{S1} A. Rey Planells and A. Espinosa Ferao, *Inorg. Chem.*, 2020, **59**, 11503–11513.

^{S2} S. E. Wheeler, K. N. Houk, P. v. R. Schleyer, W. D. Allen., *J. Am. Chem. Soc.*, 2009, **131**, 2547-2560.

Table S1: Computed zero-point corrected energy data ΔE_{ZPE} (kcal/mol) for the interconversions among CRNO isomers. Energies are referred to the respective oxazirine species (**1a-c**).

	(1a→2a)[‡]	2a	(1a→3a)[‡]	3a	(4a→3a)[‡]	4a	(3a→5a)[‡]	(1a→5a)[‡]	5a	(1a→6a)[‡]
DLPNO-CCSD(T)/def2-TZVPP	59.98	19.09	51.82	-4.05	21.82	21.56	63.09	51.92	-16.9	21.13
CASSCF(6,6)/MRACPF/def2-TZVP	62.06	24.19	52.19	4.23	23.53	25.13	62.07	50.52	-12.12	23.82
	(2a→6a)[‡]	6a	6a^t	(6a→7a)[‡]	7a	(1a→8a)[‡]	(2a→8a)[‡]	8a	(2a→9a)[‡]	9a
DLPNO-CCSD(T)/def2-TZVPP	32.36	86.27	-2.37	3.78	-62.46	118.4	118.99	78.35	42.29	46.75
CASSCF(6,6)/MRACPF/def2-TZVP	26.97	81.62	-1.58	9.35	-53.71	102.63	103.05	75.61	51.9	47.56
	(9a→10a+11)[‡]	10a+11	6a^t-10a^t+11	(9a→10a^t+11)^{mecp}	10a^t+11	(1a→12a^t)^{mecp}	12a^t	12a^s	2b	3b
DLPNO-CCSD(T)/def2-TZVPP	39.33	39.41	4.49	43.4	-6.35	9.74	-3.64	25.42	31.99	14.51
CASSCF(6,6)/MRACPF/def2-TZVP	45.04	36.15	9.34	48.52	-2.57	6.8	-2.49	1.85	34.88	19.84
	4b	5b	6b	7b	8b	9b	10b+11	10b^t+11	12b^t	2c
DLPNO-CCSD(T)/def2-TZVPP	39.50	-10.15	-67.18	-41.79	87.48	-	-50.86	0.71	0.06	18.49
CASSCF(6,6)/MRACPF/def2-TZVP	39.11	-6.68	-64.25	-36.16	81.02	-	38.03	-1.18	0.96	23.19
	3c	4c	5c	6c	7c	8c	9c	10c+11	10c^t+11	12c^t
DLPNO-CCSD(T)/def2-TZVPP	-3.62	-	-14.06	-86.70	-60.38	78.60	-	33.08	-9.14	-4.29
CASSCF(6,6)/MRACPF/def2-TZVP	3.68	-	-9.40	-78.56	-53.07	73.06	-	-17.91	-12.14	-5.53

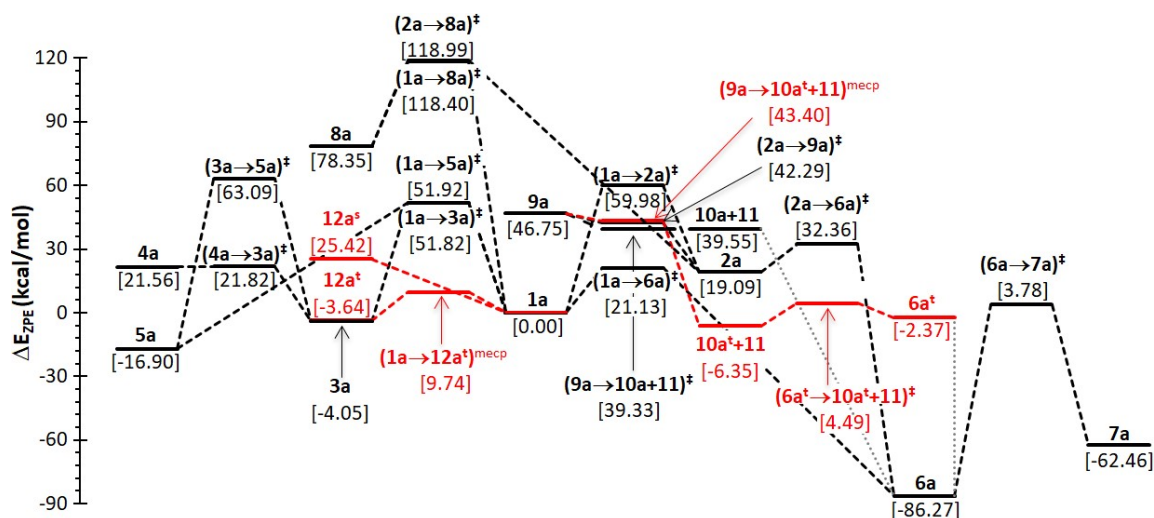


Figure S2: Computed (DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/def2-TZVP) zero-point corrected energy profile for the interconversions among CHNO isomers. Red colour indicates open-shell species.

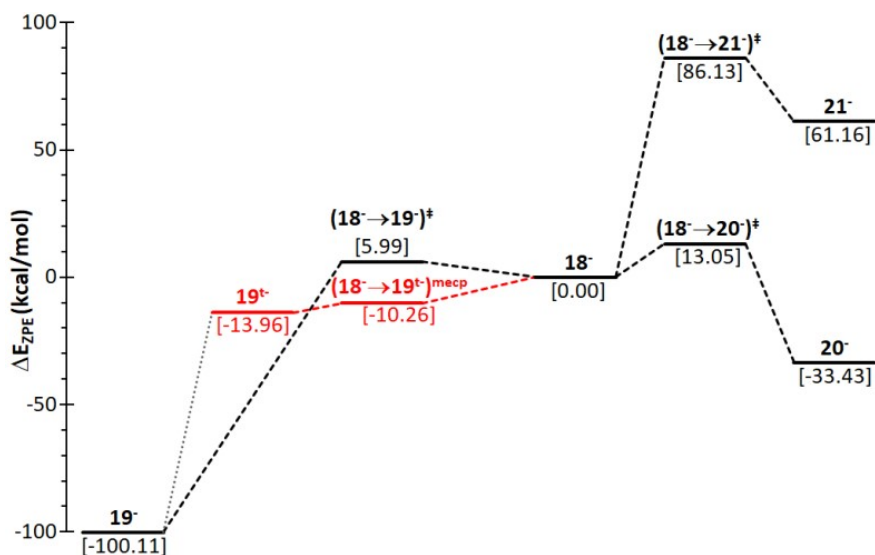


Figure S3: Computed (DLPNO-CCSD(T)/def2-TZVPP//B3LYP-D3/def2-TZVP) zero-point corrected energy profile for the interconversions of anionic CON⁻ isomers. Red colour indicates open-shell species.

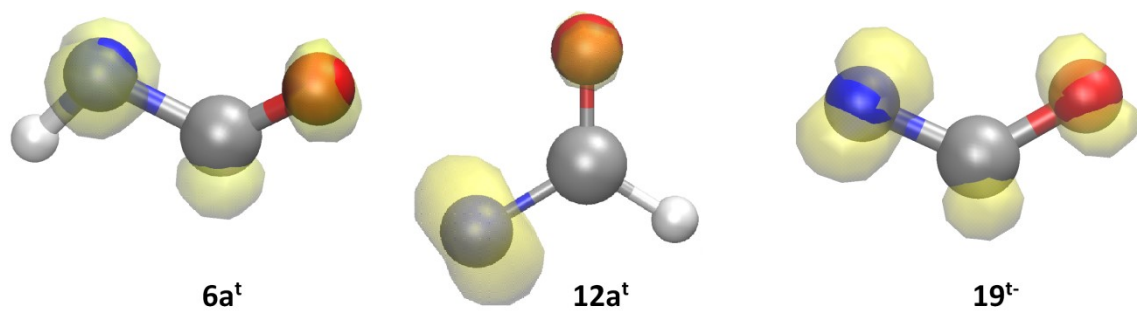


Figure S4: Computed (B3LYP-D3/def2-TZVP) spin density isosurface (0.04 au) for open-shell isomers **6a^t**, **12a^t** and **19^{t-}**.

Calculated structures

Cartesian coordinates (in Å), G correction (G-E) and ZPE (in hartrees) for TSs and minima were computed at B3LYP-D3/def2-TZVP. For TSs the imaginary frequency is given. In addition, unless otherwise indicated, electronic energies (in hartrees) are quoted using the default CASSCF(6,6)/MRACPF/def2-TZVP level and also collecting those at DLPNO-CCSD(T)/def2-TZVPP (indicated).

1a E = -168.3018986 au
E = -168.2528671 au [CASSCF(6,6)/MRACPF/def2-TZVP(-F)]
E = -168.0191660 au [CASSCF(6,6)/MRACPF/def2-SVPD]
E = -168.2974765 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.01988383 au
G_{corr} = -0.00388192 au

C	-2.02132907862173	1.49351612486192	1.85440049228218
H	-2.27454749888140	1.04136364949904	2.80775905445467
O	-2.40376664848329	2.60230450267080	1.29039738249309
N	-1.31097691401358	1.26876149296823	0.84993402077005

(1a→2a)[‡] E = -168.1972485 au
E = -168.1961331 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.014124723 au
v = -1499.02 cm⁻¹

C	-0.22024716716685	-0.53133700114497	-0.30946756795982
H	-0.74096950093380	-0.09374265438072	0.74704421246170
O	1.10985194495611	-0.13364350654646	-0.26526756845896
N	-0.14863527685546	0.75872316207215	-0.17230907604292

(1a→3a)[‡] E = -168.2134519 au
E = -168.2096129 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.014603484 au
v = -1278.88 cm⁻¹

C	0.32856657726870	0.00936855375311	0.68164443227710
H	0.05521861710143	0.99250157299159	0.06436832010400
O	-0.41720841382725	0.04273722004080	-0.86792525612668
N	0.03342321945711	-1.04460734678549	0.12191250374557

(1a→5a)[‡] E = -168.2174125 au
E = -168.2107647 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.01590972 au

$v = -732.97 \text{ cm}^{-1}$

C	-0.55404295619236	4.33350434889466	-1.75211282366991
H	-0.56538765730607	3.24701798295892	-1.82521392444690
N	0.18854340113155	5.09542594360871	-2.42079433899123
O	1.23273379236687	5.25096381453747	-1.63836399289185

(1a→6a)[‡] E = -168.2608490 au

E = -168.2607075 [DLPNO-CCSD(T)/def2-TZVPP]au

ZPE = 0.016792876 au

$v = -1267.55 \text{ cm}^{-1}$

C	0.05179852381090	-0.02851980170491	0.00000125785736
H	-0.54603160001739	-0.99559235857389	-0.00000040493317
O	1.28634367923438	0.09427621055871	-0.00000046450087
N	-0.79211060302789	0.92983594972009	-0.00000038842332

(1a→8a)[‡] E = -168.1337424 au

E = -168.1041813 [DLPNO-CCSD(T)/def2-TZVPP]au

ZPE = 0.015274465 au

$v = -720.73 \text{ cm}^{-1}$

C	-0.17001861599475	-0.96481827091374	-0.00494933601240
H	-1.13917769640238	-0.41013711313276	0.00275512461376
O	0.76624419326708	0.07818552451457	0.00529485383400
N	0.54295211913005	1.29676985953193	-0.00310064243536

(1a→12a[†])^{mecp}

E = -168.2907485 au

E = -168.2816405 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.0195637 au

$G_{\text{corr}} = -0.02426711 \text{ au}$

C	-0.40767942735362	3.30672897631472	-1.90912091710312
H	0.16255267405311	2.37578375216949	-1.90912138160010
O	0.04839176550259	4.49878110148716	-1.90912277051704
N	-1.66583307220207	3.53416980002856	-1.90912001077968

2a E = -168.2629612 au

E = -168.2666545 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.01948947 au

$G_{\text{corr}} = -0.00313578 \text{ au}$

C	-1.78064742752972	-1.07938907093976	0.43501113698866
N	-2.10498744736413	0.13811769798509	1.14328689919579
O	-0.74690004097283	-0.58828876776935	0.99106263550978
H	-2.41957679413331	-0.13536081927598	2.08171679830576

(2a→6a)[‡] E = -168.256123 au
E = -168.243125 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.017095011 au
 $\nu = -659.27 \text{ cm}^{-1}$

C	0.55958146031848	0.77331167386658	-0.27800308585432
N	-0.78212182439028	0.21636780028135	0.16276755290417
O	1.09058200114419	-0.19917564432012	0.14270951212408
H	-0.86804163707239	-0.79050382982782	-0.02747397917393

(2a→8a)[‡] E = -168.1337155 au
E = -168.103891 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.015922687 au
 $\nu = -703.23 \text{ cm}^{-1}$

O	0.76515945710124	0.07744905417473	-0.00001635686473
C	-0.16717226396723	-0.95998428432822	0.00001734651239
N	0.54330787793760	1.29473153805432	0.00000975622052
H	-1.14129507107161	-0.41219630790084	-0.00001074586818

(2a→9a)[‡] E = -168.2145269 au
E = -168.2254216 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.01521499 au
 $\nu = -213.15 \text{ cm}^{-1}$

C	-1.46702529015852	-0.33888904298160	0.66796634809205
N	0.75939066590362	-0.34016224330779	-0.79531551811219
O	-0.41569896193754	0.05398342180482	0.82340804865586
H	1.12333358619244	0.62506786448457	-0.69605887863572

3a E = -168.2955045 au
E = -168.3042721 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.020233 au
 $G_{\text{corr}} = -0.00325614 \text{ au}$

C	-0.85955314016802	1.61387695317389	-0.08486445259494
N	-1.32388621826398	2.04487474811738	-1.06786756586027

O	-1.80539361517901	2.71482021837646	-2.10898095443976
H	-2.13010874638898	2.04054842033226	-2.72851697710503

(3a→4a)[‡] E = -168.2629713 au
E = -168.2612747 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.018447646 au
 $\nu = -205.90 \text{ cm}^{-1}$

C	0.73972977710951	-0.59424516467549	0.78928798308907
N	-0.46807674011754	-0.51532229347582	0.58600683579678
O	-0.09226916127479	0.07859966041202	-0.77264426180291
H	-0.17938387571718	1.03096779773929	-0.60265055708293

4a E = -168.2609372 au
E = -168.2622129 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.01897676 au
 $G_{\text{corr}} = -0.00525445 \text{ au}$

C	-1.64562315722926	0.54408144137434	0.16528557353621
N	-1.25263371389100	1.52223678220238	0.80456280595795
O	-0.06696729602143	0.51491861623967	0.95648788302079
H	-0.24925511285831	0.11286974018361	1.82236148748504

5a E = -168.3206177 au
E = -168.3238207 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.01929082 au
 $G_{\text{corr}} = -0.00046434 \text{ au}$

C	-0.34454589354295	4.03586676319773	-1.90799549297866
H	-1.05017934830968	3.24443403236054	-1.91091010616958
N	0.44198468324965	4.88274211958656	-1.90901673572742
O	1.25458713860298	5.76386917485515	-1.90856274512432

6a E = -168.4333754 au
E = -168.4363605 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.02128412 au
 $G_{\text{corr}} = -0.00159585 \text{ au}$

C	0.96626506935932	2.83145484079621	0.80551972829010
O	2.12535651264776	2.94008477982728	0.80551971563945
N	-0.24335126668386	2.86688785792254	0.80551971658862
H	-0.85412831532321	2.06844248145397	0.80551971948183

6a^{lin} E = -168.4232549 au
 E = -168.4274772 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.02050292au
 v=-584.04 cm⁻¹

C	0.64044975208627	2.89322381353446	0.80551968681540
O	1.81328976756704	2.89322389978316	0.80551991791243
N	-0.53766412717720	2.89322372841662	0.80551925642187
H	-1.52593339247612	2.89322391826576	0.80552001885031

(6a→7a)[‡] E = -168.2827099 au
 E = -168.2871753 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.015600737 au
 v= -1629.63 cm⁻¹

C	0.13589816771447	-0.07972242492801	-0.30561285611060
N	-0.86062816930320	-0.24516485249555	-0.93901360165973
O	1.08508666591477	0.13104263232953	0.50207476424000
H	-0.36035666432604	0.19384464509403	0.74255169353033

6a^t E = -168.3022910 au
 E = -168.2991241 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.01775636 au
 G_{corr} = -0.00691705 au

C	1.06901104930134	2.47215268368481	0.80550995888422
O	2.04658722763175	3.14929125669696	0.80552587603558
N	-0.24555896811204	2.94765500399105	0.80552028706898
H	-0.87589730882105	2.13777101562717	0.80552275801122

(6a^t→10a^t+11)[‡] E = -168.2823511 au
 E = -168.285649714212 [DLPNO-CCSD(T)/def2-TZVPP]au
 ZPE = 0.01521473 au
 v= -317.13 cm⁻¹

C	1.34048698789278	2.41423654409403	0.83164098316365
O	2.17702553525212	3.18139753053226	0.79239588480217
N	-0.53730935056251	3.02272659051628	0.78610292277442
H	-0.98606117258240	2.08850929485736	0.81193908925974

7a E = -168.3890715 au
 E = -168.3985843 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.02146139 au

$G_{\text{corr}} = -0.00166105 \text{ au}$
 C -0.23641834173709 3.21081438967257 1.06452357291857
 N 0.91688640193289 3.18690705109071 1.06360184304808
 O -1.53200187281155 3.16300072654801 1.06272250172201
 H -1.91102829738425 4.05430774268870 1.09558988231134

8a E = -168.1797290 au
 E = -168.1709468 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.01821034 au
 $G_{\text{corr}} = -0.00485774 \text{ au}$

C -0.10828460909275 3.57295356066578 -1.90912127372311
 H -1.20001977822295 3.58525360356254 -1.90912127055463
 O 0.37579722475423 4.71437565650050 -1.90912126041401
 N 1.03443144256147 5.70787425927118 -1.90912127530824

9a E = -168.2240239 au
 E = -168.2208875 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.01779815 au
 $G_{\text{corr}} = -0.00590695 \text{ au}$

O -0.96284153753794 1.35480094250717 -0.26282090804500
 C -1.91091376040435 1.21502848910161 0.37106474220646
 N 0.20448259399384 1.12510133441277 -1.12515646414026
 H 0.53078959394845 2.09946800397844 -1.15239424002120

(9a→10a+11)* E = -168.2234052 au
 E = -168.228077 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.01316432 au
 $v = -41.00 \text{ cm}^{-1}$

O -1.68089104291763 1.85055412143942 0.13335026046685
 C -2.07643048155440 0.94348997008024 0.67044944088722
 N 1.22913921032957 1.19376703243244 -1.47792073205760
 H 0.38969920414248 1.80658764604781 -1.49518583929644

(9a→10a[†]+11)^{mecp} E = -168.2209691 au
 E = -168.2246971 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.01626946 au
 $G_{\text{corr}} = -0.02880679 \text{ au}$

O -1.05419975292298 1.42175750180201 -0.18318058479260
 C -1.98901316301379 1.16750464250559 0.41312205255747

N	0.31701493155335	1.10331275961215	-1.20485124236692
H	0.58771487438343	2.10182386608019	-1.19439709539795

10a E = -55.0781068 au
E = -55.06949046 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.00747381 au
G_{corr} = -0.00873648 au

N	-2.03304859424175	2.41855659000000	1.63464752000000
H	-0.99303218575825	2.41855659000000	1.63464752000000

10a^t E = -55.1397085 au
E = -55.14230774 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.00737551 au
G_{corr} = -0.00987581 au

N	-3.91241128389151	-0.28287744000000	1.03861521000000
H	-2.87033479610849	-0.28287744000000	1.03861521000000

11 E = -113.1588191 au
E = -113.1578132 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0050407 au
G_{corr} = -0.01407749 au

O	-0.48650730345425	4.49393229000000	-0.11176025000000
C	-1.61156339654575	4.49393229000000	-0.11176025000000

12a^s E = -168.3018752 au
E = -168.259891 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0198881 au
G_{corr} = -0.0038770 au

C	-0.40202269687798	3.25087700352221	-1.90912970372595
H	0.17463034816257	2.33184123629294	-1.90911691537606
O	-0.04188920542141	4.50139082904624	-1.90912365936774
N	-1.59328650586319	3.63135456113861	-1.90911480153024

12a^t E = -168.3045694 au
E = -168.3019826 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.01858447 au
G_{corr} = -0.00631822 au

C	-0.40661470439868	3.41504358419519	-1.90911571798755
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H	0.10378364494474	2.43481109947648	-1.90912329719424
O	0.20519416343714	4.48155439603754	-1.90912317704137
N	-1.76493116398321	3.38405455029079	-1.90912288777682

(6a→13a)[‡] E = -505.2501650 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0705287 au
 v = -497.87 cm⁻¹

C	-0.48785009895959	-1.71275675978757	0.00092495330424
C	1.72505634962864	0.43110975159478	0.00011179243041
C	-1.23805765839423	1.27956482765083	-0.00104319579390
N	-1.49316980483169	0.05015887173317	-0.00034971390189
N	0.78886891129243	1.26761845463499	-0.00058050457847
N	0.70297338294203	-1.31578925393083	0.00100965995654
O	-1.36030714966364	-2.49075518129588	0.00115407052782
O	-1.47266612467674	2.42507823581774	-0.00179508726755
O	2.83430412559817	0.06141786546602	0.00054720964105
H	1.38988537651103	-2.06364379334217	0.00159364757172
H	-2.48504317454505	-0.16744019148726	-0.00043268845662
H	1.09600586509863	2.23543717294618	-0.00114014343335

13a E = -505.3966456 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0806177 au
 G_{corr} = 0.0488471 au

C	-5.95987111189906	-0.76898334784478	-0.25430146818358
C	-3.81468655402400	0.46931016390181	-0.25465675658231
C	-5.95973374430978	1.70785344323494	-0.25581589103029
N	-6.58175978799531	0.46946543304219	-0.25522464344508
N	-4.57644091149765	1.62686159193010	-0.25548887959842
N	-4.57656747773926	-0.68815984334028	-0.25411816186883
O	-6.56158767635043	-1.81322124995590	-0.25401359152987
O	-6.56133074270634	2.75215510925045	-0.25658055200711
O	-2.60954806264116	0.46924375327036	-0.25444804090733
H	-4.07253406157631	-1.56232170569924	-0.25352179048819
H	-7.59090254476071	0.46951227769129	-0.25551168398513
H	-4.07228625449997	2.50095461451908	-0.25592120037385

(13a→13a')[‡] E = -505.2947448 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0751617 au
 v = -1841.81 cm⁻¹

C	-0.39790267938384	-1.14762405195413	0.00056596299664
C	1.23157837127098	0.40258097110864	0.00003821503392

C	-0.87112156533068	1.11759769416233	-0.00084300291233
N	-1.30946876560151	-0.19016524179067	-0.00025755858831
N	0.90428398519048	-0.89261096706232	0.00073357957829
N	0.41129125653533	1.45639273998276	-0.00074447837292
O	-0.81136630702322	-2.40478899765719	0.00124823374296
H	-0.02030779643076	-2.96654847635205	0.00176810572770
O	-1.92651849022957	1.82263423560152	-0.00141989082215
H	-2.37987567186441	0.52701543961248	-0.00083694951405
O	2.53412178610636	0.65544682510351	0.00014788691758
H	2.63528587676083	1.62006982924512	-0.00040010378732

13a' E = -505.3559772 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0799845 au
 G_{corr} = 0.0485088 au

C	-0.39208420137462	-1.09861208288244	0.00055563149719
C	1.22268134357151	0.43100256029918	0.00000721160930
C	-0.92278212076755	1.25885140439554	-0.00098929060572
N	-1.30647139243906	-0.12192782124799	-0.00022123806379
N	0.89018863017767	-0.88562222077574	0.00069988126628
N	0.42930877207051	1.46755531679115	-0.00076314911103
O	-0.87725531973677	-2.33545025054537	0.00119899934396
H	-0.11910103226722	-2.94106556592663	0.00169184604267
O	-1.78485983032285	2.10140492353553	-0.00158008607290
H	-2.29392701286402	-0.33332794064845	-0.00030007154888
O	2.53620457387127	0.64500661818154	0.00017188985121
H	2.66033659008112	1.60698305882369	-0.00035562420828

(13a'→13a'')[‡] E = -505.3010055 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0749939 au
 ν = -1871.21 cm⁻¹

C	-0.35421779968099	-1.10474446646278	0.00057930246752
C	1.37255608063194	0.27696294145329	0.00014120413296
C	-0.77826558729241	1.30270269589097	-0.00093729523915
N	-1.20974681510718	-0.06908944130156	-0.00019381009397
N	0.57784665205955	1.37805231584251	-0.00068765574463
N	0.94783887424064	-1.00153856380523	0.00079589157254
O	-0.92904094982765	-2.29937020663364	0.00114172490080
O	-1.59126310024697	2.18904662496097	-0.00165819174490
O	2.56756153593461	0.70446998958889	0.00015699225806
H	-0.21941822249904	-2.96159109097510	0.00164952873483
H	-2.20653026007796	-0.23010073603559	-0.00031260201873
H	1.82267959186546	1.81519993747729	-0.00067508922534

13a'' E = -505.3715927 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0800630 au
 G_{corr} = 0.0483871 au

C	-0.32896362477842	-1.10391814442830	0.00058054698533
C	1.53906998018311	0.22956523221266	0.00020153909107
C	-0.72460933061174	1.26730976086506	-0.00089622232410
N	-1.18852629803682	-0.05074454131790	-0.00022707120118
N	0.64538959418434	1.32527178986840	-0.00063427971286
N	0.95201025318531	-1.02736044814967	0.00082194345167
O	-0.95240208534956	-2.28095569372518	0.00112984280899
O	-1.46897139595632	2.21614120613445	-0.00161400555427
O	2.72712801070444	0.42486751595284	0.00032936351713
H	-0.26504715410726	-2.96558823753485	0.00167535368912
H	-2.18712446037774	-0.19340597800515	-0.00037353295397
H	1.06064551096065	2.24567753812765	-0.00108747779695

(13a''→14a)[‡] E = -505.3176100 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0751531 au
 ν = -1883.20 cm⁻¹

C	-0.53701206545234	-1.13489038125433	0.00055549418407
C	1.50106705811209	0.08098951171517	0.00026813177846
C	-0.72507300279980	1.24949850619865	-0.00088418877190
N	-1.30669342946638	-0.03389460743839	-0.00027272589470
N	0.65037724565239	1.21568777177501	-0.00056914466747
N	0.79328591745427	-1.09914500344368	0.00082374172611
O	-0.90389026388185	-2.35101246594852	0.00120292032595
O	-1.39355732575633	2.25052278323091	-0.00159902840417
O	2.69686997491749	0.20018060201399	0.00044334197994
H	0.42440572148216	-2.39749850545241	0.00150285244484
H	-2.31396531792357	-0.09298917043791	-0.00048539371728
H	1.11418548766188	2.11255095904151	-0.00098600098385

(7a→14a)[‡] E = -505.1754956 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0709824 au
 ν = -574.36 cm⁻¹

N	-1.54907074366691	0.31144950384731	0.00000212419036
C	-1.37123205771312	-0.85556972962553	0.00000076758200
O	-1.89147762771899	-2.04309292555906	-0.00000036090342
H	-1.14052008046841	-2.66727543522772	-0.00000118396188
N	0.50471021194101	-1.49715986107987	-0.00000034713943
C	1.42652117283143	-0.75974321701685	0.00000008332542
O	2.71502023426275	-0.61658316328993	0.00000073615128

H	2.88018968933427	0.34584414941777	0.00000016282200
N	1.04431662117466	1.18582333760036	-0.00000065423491
C	-0.05528338037372	1.61529284448472	-0.00000033913795
O	-0.82356120089424	2.65961020743179	-0.00000096423707
H	-1.73961283870874	2.32140428901702	-0.00000002445638

14a E = -505.3585087 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.0803730 au

G_{corr} = 0.0491488au

C	-5.61818808008737	6.31578868590625	0.03659415106329
C	-3.54842319801581	7.11840781750522	0.18275274239121
C	-5.25254072641922	8.49810453626955	-0.19485844670471
N	-6.14853299813893	7.51322861546614	-0.17780908607787
N	-4.32805874212216	6.04537960453887	0.22493721664488
N	-3.94264223101986	8.37366339077496	-0.02272783597432
O	-6.46821794309869	5.29320930387458	0.06467164108445
H	-5.94464409785174	4.49397124579717	0.22822076764821
O	-5.70393286125159	9.73186664742941	-0.40322540068093
H	-6.66501181145743	9.66737467507847	-0.51117819752431
O	-2.24809998822473	6.90716810974908	0.36563848919959
H	-1.80946523231227	7.76956284760999	0.30764874893054

(6a→15a)[‡]

E = -505.1584140 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.0711852 au

v = -655.74 cm⁻¹

C	-0.71267955727902	-1.38801714178338	0.02181681771459
C	1.22652391496898	1.45191557578232	0.12842058457994
C	-0.86351102621718	1.13608712188513	-0.15550871566796
N	-1.34793387887918	-0.08564865043374	-0.03003103335093
N	0.50807662631386	-1.40949784242201	-0.49639367585984
O	-1.41226400604080	-2.28573262475227	0.46046851077143
O	-1.29121439608485	2.21731472390731	-0.30852706657925
H	0.99426294731823	-2.23695216770232	-0.15168610941736
H	-2.33215479366708	-0.14238755957665	0.22482979356521
O	1.31642498381869	2.62710191476366	0.12217667474068
N	1.58361218985771	0.27609813956354	0.34984615279834
H	2.33085699589064	-0.16028148923160	-0.16541193329485

15a E = -505.3042108 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.0789892 au

G_{corr} = 0.04698839 au

C	-0.69162021271635	-1.25678193526211	0.00520500427520
C	0.80089291134892	1.23154829855310	-0.02221724671505
C	-0.73342840681979	1.23519395342103	0.02423166950581
N	-1.31925609357902	-0.01733100012507	-0.04106585836669
N	0.68060092443072	-1.21202202493293	-0.10797469190230
O	-1.29965089044205	-2.29548220546475	0.11510642567158
O	-1.37132414518227	2.25014368727263	0.07679616127946
H	1.13510716991878	-1.99815072194138	0.33531250538706
H	-2.33077409273142	-0.04880451574533	-0.01149153779788
O	1.44314069799532	2.24727528269474	-0.11972343587910
N	1.38633558866033	-0.00486561940820	0.05133719613921
H	2.34110693883248	-0.04865902884633	-0.27855451456364

(6a→16a)[‡] E = -336.8231112 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.04569825 au
v = -570.13 cm⁻¹

N	0.10317440403745	2.94005653988558	-0.99274198657801
H	-0.69062460253622	3.55617172360602	-1.11650595160502
N	1.81560176192155	1.51487497208458	-0.71962108429703
H	2.60864549857354	0.90800027022407	-0.55208879414533
C	2.00601366823774	2.77233925132749	-0.79838498080395
C	-0.09319114291571	1.68556935522016	-0.89250792594448
O	-0.72367833044037	0.70580598766993	-0.85603838087108
O	2.63431986312191	3.75435771998173	-0.81557338575494

16a E = -336.8782547 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.05018035 au
G_{corr} = 0.02202314 au

N	0.21981745044831	2.91720794203064	-0.86031853698264
H	-0.40092865322203	3.55125364021585	-1.34007495002040
N	1.69527451908885	1.54206767415439	-0.82559696867145
H	2.31594896359015	0.90805897057463	-0.34569948680680
C	1.63569051573093	2.95946384869391	-0.75557345634142
C	0.27938940744893	1.49982166560358	-0.93029912943643
O	-0.52528995636225	0.63387241539185	-1.03400396319342
O	2.44035887327709	3.82542966333513	-0.65189599854743

(5a→17a)[‡] E = -504.8385143 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0642533 au
v = -828.36 cm⁻¹

C	-1.15829079008246	0.85341924754743	0.50889047888366
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N	-0.24595468498199	1.63685741059558	0.48707883109719
O	0.24814808561517	2.74247445227926	0.65220410642148
C	1.38380016503300	0.61912690787482	-0.17490731726414
N	1.55733410544343	-0.52086767415849	-0.51745604150679
O	2.24736079448825	-1.44197256862846	-0.93001855135494
C	-0.22329418207901	-1.47397908208864	-0.32932739023683
N	-1.31327993205191	-1.11474659846612	0.03081445243612
H	-2.20928809356506	0.80584033907046	0.75424188166945
O	-2.49768195965614	-1.29773747719095	0.27214066458447
H	0.28638401271507	-2.35601018070579	-0.68898686313938
H	1.92476247912165	1.54759522387089	-0.06467425159029

17a E = -505.0534103 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.0761698 au

G_{corr} = 0.0449806 au

C	-3.07535985281192	0.57819439314978	0.81348054665169
N	-2.28558891243032	0.60085557492204	-0.29017962752120
O	-2.24961534466379	1.62864867315460	-1.02264672217728
C	-1.53545786096601	-0.48587888538018	-0.60407072069849
N	-1.57130198009777	-1.59186815079085	0.18199491385531
O	-0.87233580180556	-2.60126083692377	-0.11265347905549
C	-2.36177920251364	-1.60854393983915	1.28531625902561
N	-3.11626556847975	-0.52551053546267	1.60244969424670
H	-3.67036592889570	1.43680076426469	1.06313473300921
O	-3.85359854085103	-0.54466150047199	2.62714653149029
H	-2.39304435953863	-2.48330422362540	1.90777392941076
H	-0.91169449694586	-0.47108343299710	-1.47831636823710

1b E = -207.5459548 au

E = -207.5546345 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.04806949 au

G_{corr} = 0.02155320 au

C	-2.02763413032465	1.42729196919709	1.92715709292705
O	-2.33945413821240	2.60383679739116	1.44675217390460
N	-1.42187087664983	1.21900538526564	0.85029409476579
C	-2.33844451709199	0.78407389062204	3.21212405874346
H	-1.93042629091305	1.39201134735744	4.02174098952329
H	-3.42187648536732	0.73702366404124	3.33524391121797
H	-1.91617221144074	-0.21849215387462	3.25235737891782

2b E = -207.4893261 au

E = -207.5026112 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.04703287 au

G_{corr} = 0.02066463 au

C	-1.83336873635980	-0.93343654583831	0.26436192965937
N	-2.13758362250106	-0.31196387727060	1.31127273376937
O	-0.66942642404626	-0.49108448881828	1.12371328042572
C	-2.84104816117606	0.32843759645915	2.36039051118674
H	-2.62086044482406	-0.16442238852745	3.30932762655009
H	-2.54931342393200	1.37902587468987	2.41525810084064
H	-3.90600493716074	0.24893433930561	2.13781669756808

3b E = -207.5152314 au

E = -207.5324076 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.04896734 au

G_{corr} = 0.02233808 au

C	-0.66476666847099	1.77215130072839	-0.04832544572994
N	-1.25621542280429	2.09596623823244	-1.00433147199521
O	-1.91420584014355	2.56520864352626	-2.04758846841957
C	-2.28470191419105	1.49184995031023	-2.94925150424596
H	-1.38864201947019	0.98520682879360	-3.30653706144793
H	-2.79935766330750	1.99253458317660	-3.76442217169529
H	-2.94755109161243	0.79431920523246	-2.43805753646608

4b E = -207.4821473 au

E = -207.4902111 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.04659561 au

G_{corr} = 0.02032906 au

C	-1.53330435662209	-0.56051696914717	0.94544050562182
N	-2.52672908603957	-0.22973279746130	1.43487448840367
O	-0.44975073534983	-0.94557616169557	0.36996520833938
C	0.78433434383605	-0.59204217503281	1.05840010465893
H	0.85744938878985	0.49131700889518	1.14088758198080
H	0.79668498674918	-1.05619264763193	2.04339437563012
H	1.58017654863639	-0.98676636792638	0.43506683536527

5b E = -207.5578098 au

E = -207.5720235 au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.04928412 au

G_{corr} = 0.02286556 au

C	-0.54451137269013	4.27938521467067	-1.90779781776504
N	0.43098870392561	4.89931283527845	-1.90591452235010
O	1.45222831703041	5.54832442510020	-1.90376524762395
C	-1.77183186779850	3.49607641880245	-1.91097936690222
H	-2.37549772669307	3.72922910618236	-2.79030703916574
H	-1.54670063947176	2.42787067939122	-1.92391741113963
H	-2.36740741430253	3.70942040057454	-1.02116743505327

6b E = -207.6507767 au
E = -207.6641147 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.05049626 au
G_{corr} = 0.02371572 au

C	1.04170135876911	2.86978311990100	0.80551882186050
O	2.17150143993012	3.18249569706539	0.80550680375744
N	-0.13906706627668	2.67686225224424	0.80553579762926
C	-1.07709957505259	1.58623834975811	0.80552244034388
H	-2.08808601746815	1.98916267596401	0.80570807249848
H	-0.95181823155710	0.96469248140848	-0.08321522633039
H	-0.95158317834471	0.96445614365877	1.69406137024084

7b E = -207.6058791 au
E = -207.6235298 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.05036542 au
G_{corr} = -0.00166105 au

C	-0.23828902192715	3.19257913088517	1.06387373574314
N	0.91599655023461	3.13443286598369	1.06471854914238
O	-1.52400711493021	3.21898266308286	1.06156216462071
C	-2.11950149083514	4.54765417358192	1.11336043663790
H	-1.81342766841069	5.11741517830476	0.23720387683626
H	-3.19137450018652	4.37864372861876	1.10991305404463
H	-1.80858335394490	5.05022284954281	2.02807591297498

8b E = -207.4158252 au
E = -207.4142088 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.04704898 au
G_{corr} = 0.02028830 au

C	-0.21493091941419	3.54623099118956	-1.90964090327531
O	0.30690294415262	4.66352470813109	-1.90908491267099
N	0.96845549562585	5.66938975585489	-1.90864952067328
C	-1.71210142688655	3.47899126355312	-1.90922792397508

H	-2.12162430221207	3.97408732871217	-2.79649538918354
H	-2.02844548031049	2.43970393118984	-1.91070575150415
H	-2.12091061095517	3.97123609136931	-1.02004443871765

10b E = -94.32325545 au
E = -94.4745968 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0397545 au
G_{corr} = 0.0178485 au

N	-1.01105014989470	2.48575056909570	2.41271033459398
C	-0.28914645905494	2.63450396407486	1.38659606731504
H	-1.30061175438286	1.51237778566805	2.52605342347537
H	-0.00343423903166	1.83088473680493	0.69972937267578
H	0.08904021236417	3.62926594435644	1.14814841193983

10b^t E = -94.3826441 au
E = -94.3893284 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0366605 au
G_{corr} = 0.0134641 au

N	-1.85433125550993	2.73286244986078	2.19386366500947
C	-0.59325893183238	2.42614812705311	1.64795108699247
H	0.20651532340176	2.96679895763016	2.17692449530894
H	-0.38454091226668	1.34802438582289	1.72555593732893
H	-0.54789815379274	2.70587975963302	0.58413572536016

12b^t E = -207.5432697 au
E = -207.5533818 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.04691315 au
G_{corr} = 0.01909046 au

C	-0.33870242686289	3.37868671836396	-1.90916382135825
O	0.18179972548886	4.49289639986801	-1.90939973767844
N	-1.71245244843832	3.32926756462051	-1.90874656773578
C	0.41912011349987	2.07836064498067	-1.90919294678115
H	0.15328809919558	1.49038904417084	-1.02827709746297
H	0.15074083931372	1.48874227030809	-2.78821731060413
H	1.48848736780318	2.28040416768790	-1.91085139837928

1c E = -504.9455528 au
E = -504.958993 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.02527087 au

$G_{\text{corr}} = -0.00528488$ au

C	-2.01594706044268	1.47805216041094	1.81347381947748
O	-2.26186752697014	2.63185794996228	1.28605176891343
N	-1.41659526556269	1.12495958760934	0.77454861454104
C	-2.37275371489532	0.90083353847728	3.16854578903193
F	-1.90535519224529	-0.34426286806536	3.26683318556954
F	-3.69898615019715	0.88724045315966	3.31832403417630
F	-1.83706482968672	1.64729804844585	4.13673376829026

2c

$E = -504.9076466$ au

$E = -504.9285786$ au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.02432172 au

$G_{\text{corr}} = -0.00573660$ au

C	-1.46057799128342	-1.05611202026665	0.29023216506596
N	-2.24863201378464	-0.13616517014413	1.11741278877260
O	-0.73573619798223	-0.19976783851897	0.87826653352595
C	-2.55006945374843	-0.62924012959566	2.45303034703973
F	-1.82826081328713	-1.69051692737730	2.83180385039836
F	-3.83898263384173	-0.96499218421545	2.42655600090905
F	-2.36687464607242	0.33651693011816	3.35006072428834

3c

$E = -504.9401457$ au

$E = -504.965219$ au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.02572968 au

$G_{\text{corr}} = -0.00480922$ au

C	-1.22956335167660	1.62019015203786	-0.06574145374096
N	-1.35623503654036	2.17487622714371	-1.08905100425486
O	-1.44798745509943	2.62600479707281	-2.33486352611695
C	-1.83792959875230	3.98116097284799	-2.37291732523555
F	-0.94959248776752	4.75071689823150	-1.76197221322461
F	-3.02199069598110	4.15223079325195	-1.80488115869010
F	-1.89521632418267	4.27456095941415	-3.65622297873694

5c

$E = -504.9618998$ au

$E = -504.9827705$ au [DLPNO-CCSD(T)/def2-TZVPP]

ZPE = 0.02663509 au

$G_{\text{corr}} = -0.00486664$ au

C	-0.50475740414075	4.30418539354324	-1.90766520843914
N	0.47177871047733	4.92530638502773	-1.90581037032903
O	1.47598181112503	5.56368810318656	-1.90375462005320

C	-1.73657671753896	3.51854919104714	-1.91086476787997
F	-2.48509299523225	3.79949904842018	-2.98935954830215
F	-1.46881910626420	2.20320675182808	-1.92679716131948
F	-2.47524629842617	3.77518420694694	-0.81959716367696

6c E = -505.0732803 au
E = -505.0996842 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.02780237 au
G_{corr} = -0.00283145 au

C	1.02317914739665	2.86688333533088	0.80552885378589
O	2.16125472687271	3.07178168883198	0.80566793007780
N	-0.18757270911688	2.78783754789323	0.80535168183212
C	-1.02772256007180	1.66485117147334	0.80548756600176
F	-2.29951611332820	2.05899303521579	0.80583894166632
F	-0.83231041292179	0.89175610088148	-0.27882815741127
F	-0.83176334883070	0.89158784037329	1.88959126404740

7c E = -505.0320341 au
E = -505.0571288 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.02718689 au
G_{corr} = -0.00303259 au

C	-0.20440811509960	3.18550512932943	1.06355463765755
N	0.94216307336704	3.08025786577779	1.06076349325584
O	-1.50552658316990	3.22745839440031	1.06389862068587
C	-2.10417645305970	4.49822867732139	1.11172825856199
F	-1.75363159349442	5.22194580650001	0.05723034970452
F	-3.40298606012088	4.28435229479010	1.10572032063009
F	-1.75062086842254	5.14218242188093	2.21581204950413

8c E = -504.9618656 au
E = -504.8333532 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.02488509 au
G_{corr} = -0.00576733 au

C	-0.12355662804657	3.59291381625626	-2.06101639869839
O	0.39163219842360	4.70804545456435	-1.89459197898218
N	1.05079888024642	5.68568264864502	-1.76565038566611
C	-1.63040535556604	3.59593326100799	-1.93888637893910
F	-2.03330983633691	4.05407223446940	-0.73593491526646
F	-2.20157022591446	4.37741691354915	-2.87755252886280
F	-2.09430683280603	2.35755949150781	-2.09021629358495

10c E = -391.8101904 au
 E = -391.8211279 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0171697 au
 G_{corr} = -0.01034153 au

N	-1.01827963156225	2.59858132885160	2.45937572275736
C	-0.30251434981564	2.67564376544750	1.42021816464633
F	-1.42117818994737	1.27081790963564	2.62731646021225
F	0.03614105954958	1.71942618421521	0.60413184144776
F	0.19062872177570	3.82831381185002	1.06219542093630

10c^t E = -391.8014699 au
 E = -391.8111298 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0156178 au
 G_{corr} = -0.0126405 au

N	-1.92116557366918	2.73103034917503	2.20492519862824
C	-0.62512747364079	2.43359314666137	1.66164092014946
F	0.31919419281150	3.11119778868401	2.32636656161403
F	-0.37027755139662	1.12341317844698	1.76576617079615
F	-0.57613752410487	2.78047921703257	0.36973205881208

12c^t E = -504.9533687 au
 E = -504.9648335 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.02427625 au
 G_{corr} = -0.00737850 au

C	-0.38442479762729	3.44395336982694	-1.90920057906719
O	0.17221727022042	4.53083960009979	-1.91056643077397
N	-1.74498078467804	3.35208513438113	-1.90754194573405
C	0.40757039917773	2.10617783988562	-1.90916313647741
F	0.08919524139065	1.38814116047570	-0.82100851605953
F	0.08713930925392	1.38681284374612	-2.99582318448231
F	1.71556463226262	2.33073686158469	-1.91054508740551

18^t E = -167.7144504 au
 E = -167.7133615 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.00654035 au
 G_{corr} = -0.01708263 au

O	1.46424999817258	-0.00259487290743	0.00000000000000
C	0.03944719974914	0.37299379644463	0.00000000000000
N	0.69112962207829	1.44093970646280	0.00000000000000

(18⁻→19⁺)[‡] E = -167.7057207 au
 E = -167.7029512 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.005671401 au
 v = -645.80 cm⁻¹

O	-1.00060059785998	-0.00000000045221	-0.31665957799478
C	0.09574651052405	0.00000000088133	0.61715097621116
N	0.90485408733593	-0.00000000042912	-0.30049139821638

(18⁻→19^t)^{mecp} E = -167.7356606 au
 E = -167.7304809 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.00731264 au
 G_{corr} = -0.03626161 au

N	-1.81943340981345	-1.30451216162390	0.30485795534864
C	-2.95679896678547	-1.20155988239870	0.99607117062669
O	-3.99334154340102	-1.30603890597738	0.29449946402467

(18⁻→20⁺)[‡] E = -167.6893385 au
 E = -167.6917866 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.005759451 au
 v = -488.97 cm⁻¹

O	1.07283547272580	0.33365728143010	-0.09115251257505
C	-0.71491087707728	-0.49863518595256	0.51955013201424
N	-0.35792459564852	0.16497790452247	-0.42839761943919

(18⁻→21⁻)[‡] E = -167.5801327 au
 E = -167.5745899 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.00501813 au
 v = -781.74 cm⁻¹

O	-0.13353624094761	-0.56707160922127	-0.00010131972262
C	-1.26312644789502	-0.48254827477322	0.00005174552758
N	1.39666268884263	1.04961988399450	0.00004957419504

19⁻ E = -167.8714103 au
 E = -167.877151 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.01079919 au
 G_{corr} = -0.01050774 au

N	-1.72338041942404	-1.27070364800725	0.53180952702224
C	-2.91004476171998	-1.27070365431313	0.53180953642223
O	-4.13614873885597	-1.27070364767962	0.53180952655553

19^{t-} E = -167.7219703 au
 E = -167.7366733 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0076004 au
 G_{corr} = -0.01685357 au

N	-1.77758014512504	-1.29812975570506	0.34771445071865
C	-2.94290156353296	-1.21362065895732	0.91509021306724
O	-4.04909221134197	-1.30036053533761	0.33262392621410

20⁻ E = -167.7653608 au
 E = -167.7685447 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0084541 au

C	-2.16892874782373	0.36969544148667	0.58683908796954
N	-1.14762209593576	0.84515394648123	0.23798061243646
O	-0.05366420624051	1.35436208203210	-0.13557390040599

21⁻ E = -167.620753 au
 E = -167.6165984 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.00724236 au

C	-3.79796875552597	-0.81708829983059	-0.14345466550189
O	-2.76053326559232	-0.21557552909980	-0.14345470922793
N	-1.65611595888171	0.42517286893039	-0.14345466527018

HN=CH₂ E = -94.4642650 au
 E = -94.4383343 au [CASSCF(6,6)/MRACPF/def2-TZVP(-f)]
 E = -94.3160648 au [CASSCF(6,6)/MRACPF/def2-SVPD]
 E = -94.4744532 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0397557 au
 G_{corr} = 0.0188872 au

N	-0.09021966959467	0.22283980925514	-2.20074106045172
H	0.60360340787980	0.15710802129276	-2.94808763703110
C	0.45537872755658	0.46202435149130	-1.08671943223383
H	-0.17440039988956	0.55735517074328	-0.20146197103517
H	1.53234125404786	0.58408736721751	-0.92981463924817

HN=CH₂^{lin} E = -94.4153297 au
 E = -94.4256171 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0365536 au
 G_{corr} = 0.01475828 au
 ν = -1201.53 cm⁻¹

N	-0.91256687213434	0.51944329304643	0.51842333252416
H	-1.77593527209610	0.61242684374653	0.98886227793977
C	0.16373384277842	0.40363138065795	-0.06801585837733
H	0.94463379168167	1.18900828648112	-0.06089974161023
H	0.44126934977035	-0.49541673393203	-0.65212039047637

H₂N-OH E = -131.5284565 au
E = -131.4925516 au [CASSCF(6,6)/MRACPF/def2-TZVP(-F)]
E = -131.3139371 au [CASSCF(6,6)/MRACPF/def2-SVPD]
E = -131.5430685 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0400994 au
G_{corr} = 0.0186706 au

N	1.24437866820585	0.27251657172752	-0.20714456370169
H	1.68846390134938	0.69667978298425	0.60371941579520
H	1.67206729865746	0.70554163067655	-1.02209326593829
O	1.75512517082417	-1.07761902607584	-0.22000145156028
H	0.94962125096314	-1.60633423931248	-0.21292392459495

H₃C-OH E = -115.539093713354 au
E = -115.5080329 au [CASSCF(6,6)/MRACPF/def2-TZVP(-F)]
E = -115.3534743 au [CASSCF(6,6)/MRACPF/def2-SVPD]
E = -115.5548116 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0509757 au
G_{corr} = 0.02922996 au

O	1.59594943204642	-1.05066575113525	-0.51129554994570
H	1.09112213666446	-1.58759038742931	0.10752232106756
C	1.27030531157481	0.31653898831653	-0.29972202631816
H	1.53371584360337	0.65289345081245	0.70957520546448
H	1.85287001522521	0.89373059702188	-1.01666515394851
H	0.20769577088572	0.52035411241369	-0.47439047631968

1a^{N=C}_{cleav} E = -262.8340557 au
E = -262.7578704 au [CASSCF(6,6)/MRACPF/def2-TZVP(-F)]
E = -262.4094956 au [CASSCF(6,6)/MRACPF/def2-SVPD]
E = -262.8539453 au [DLPNO-CCSD(T)/def2-TZVPP]
ZPE = 0.0660651 au
G_{corr} = 0.0389637 au

C	-1.89165238627027	0.85608931554385	1.18647562735233
H	-1.27212644096377	1.74820391689657	1.22999764061995
H	-2.96814467210790	0.92673274371733	1.27407288636486
C	0.49751704963069	-1.52040850074767	0.77356180329393

H	-0.27790472269965	-2.28689167452705	0.74849782020709
N	-1.41844492863294	-0.30668481035181	1.03409835258648
N	1.74124173641913	-1.64850302104789	0.67695021513021
H	1.99152871627263	-2.62596367180310	0.56035768124163
O	-0.01788426164792	-0.26702020768023	0.93489919320352

1a^{N-O}_{cleav} E = -299.8840940 au
 E = -299.7973161 au [CASSCF(6,6)/MRACPF/def2-TZVP(-F)]
 E = -299.3921144 au [CASSCF(6,6)/MRACPF/def2-SVPD]
 E = -299.909716807193 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.0657479 au
 G_{corr} = 0.0374562 au

C	-1.72391026450479	-0.30921056415999	2.47269817377589
H	-2.70263113583619	-0.19318171466770	2.92966362566438
N	-1.14142887861577	0.54556557641560	1.74801444256316
N	-1.98994048514265	-2.43262148220214	3.28860123786815
H	-2.02085446718917	-3.17532271159041	2.59284554866302
H	-1.47597712491998	-2.80287196537118	4.08406704188007
O	-1.93044092420207	1.71370936774331	1.64893714988949
H	-1.39674854892092	2.27008439709863	1.07169279476220
O	-1.07441591066845	-1.47353473326612	2.72690399493365

1a^{N-O}_{cleav} E = -283.8921073 au
 E = -283.8133532 au [CASSCF(6,6)/MRACPF/def2-TZVP(-F)]
 E = -283.4330776 au [CASSCF(6,6)/MRACPF/def2-SVPD]
 E = -283.9237826 au [DLPNO-CCSD(T)/def2-TZVPP]
 ZPE = 0.07680458 au
 G_{corr} = 0.04856208 au

C	-2.08423223513640	3.12049130094136	-1.26293270403419
H	-1.98685495899169	3.39128894640082	-0.20859120677925
H	-1.57187072218393	3.86504556782725	-1.87758322508388
H	-3.13693594090712	3.07215388938139	-1.53895333268649
O	-1.56998053737580	1.81957741175263	-1.50328729976599
O	1.59702517546055	0.45539219773059	-1.11419569391190
H	1.83324826853673	-0.44487483903566	-1.35925950876978
C	0.29044434970944	0.66701186170009	-1.39578731405272
H	-0.28330244385688	-0.15684967026606	-1.81868104875955
N	-0.20801882525490	1.80348676356758	-1.15559146615625