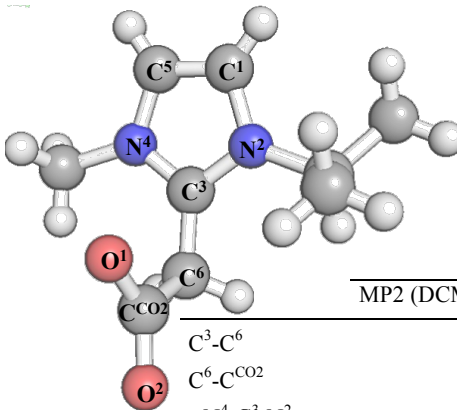


**Computationally Designed 1,2,4-Triazolylidene-Derived N-Heterocyclic
Olefins for CO₂ Capture, Activation and Storage**

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Table S1. Calculated and experimental parameters for a selected NHO-CO₂ system. The experimental values were taken from the structure described in Ref. 7. Bond distances are given in Å and angles in °.



	MP2 (DCM)/6-31+G(d,p)	Expt.
C ³ -C ⁶	1.478	1.479
C ⁶ -C ^{CO2}	1.568	1.549
∠N ⁴ -C ³ -N ²	107.00	107.58
∠O ¹ -C ^{CO2} -O ²	129.65	127.67
∠N ² -C ³ -C ⁶ -C ^{CO2}	75.31	92.84
∠N ⁴ -C ³ -C ⁶ -C ^{CO2}	95.38	81.92

Table S2. Values of $\Delta G^\ddagger$ and ΔG^{RXN} (in kcal mol⁻¹) for the reference and improved trNHOs-mediated processes.

	$\Delta G^\ddagger$	ΔG^{RXN}
trNHO (reference)	15.0	4.0
trNHO-1e-N ² -1e-N ⁴	15.3	3.4
trNHO-1e-N ² -1j-N ⁴	16.7	1.1
trNHO-1e-N ² -1i-N ⁴	15.6	-0.2

The relative energies described in Table S2 were obtained using the $G_{\text{corrected}}^{\text{DLPNO-CCSD}(T)}$ energies as follow:

$$G_{\text{corrected}}^{\text{DLPNO-CCSD}(T)} = E_{\text{SP}}^{\text{DLPNO-CCSD}(T)} + (E_{\text{MP2(DCM)}/6-31+G(d,p)} - E_{\text{SP}}^{\text{MP2}/6-31+G(d,p)}) + G_{\text{therm}}^{\text{MP2(DCM)}/6-31+G(d,p)}$$

$G_{\text{therm}}^{\text{MP2(DCM)}/6-31+G(d,p)}$ contains all contributions for thermal correction. The temperature taken is 298.15 K.

Table S3. Values of $\Delta E^\ddagger$ and ΔE^{RXN} in kcal mol⁻¹ obtained at M06-2X (DCM)/6-31+G(d,p), B3LYP-D3 (DCM)/6-31+G(d,p) and wB97X-D (DCM)/6-31+G(d,p) level of theories. Values are for selected trNHOs-mediated processes. For completeness, the DLPNO-CCSD(T) values are also included.

		M06-2X	B3LYP-D3	wB97X-D	DLPNO-CCSD(T)
trNHO (reference)	$\Delta E^\ddagger$	0.9	0.2	2.4	5.5
	ΔE^{RXN}	-14.7	-12.9	-14.8	-6.5
trNHO-1e-N ² -1e-N ⁴	$\Delta E^\ddagger$	-0.4	-1.6	0.8	4.3
	ΔE^{RXN}	-16.9	-15.6	-17.4	-8.8
trNHO-1e-N ² -1j-N ⁴	$\Delta E^\ddagger$	-0.3	-1.7	1.4	5.3
	ΔE^{RXN}	-19.2	-17.9	-19.5	-11.7

The main text contains more descriptions about these selected systems. The relative energies described in Table S3 were obtained using the $E_{\text{corrected}}^{\text{DFs}}$ energies as follow:

$$E_{\text{corrected}}^{\text{DFs}} = E^{\text{DFs}(\text{DCM})/6-31+G(d,p)} + \text{ZPE}^{\text{DFs}(\text{DCM})/6-31+G(d,p)}$$

with $\text{DFs} = \text{M06-2X, B3LYP-D3 and wB97X-D.}$

In the sequence, optimized coordinates for all chemical systems obtained at MP2(SMD,DCM)/6-31+G(d,p) level of theory are provided.

Chemical systems and their optimized coordinates:

Frames and Labels

1 CO₂

2 NHO

3 NHOvdw

4 NHOts

5 NHOadd

6 trNHO

7 trNHOvdw

8 trNHOts

9 trNHOadd

10 trNHO-1e-N2

11 trNHOvdw-1e-N2

12 trNHOts-1e-N2

13 trNHOadd-1e-N2

14 trNHO-1d-N2

15 trNHOvdw-1d-N2

16 trNHOts-1d-N2

17 trNHOadd-1d-N2

18 trNHO-1h-N2

19 trNHOvdw-1h-N2

20 trNHOts-1h-N2

21 trNHOadd-1h-N2

22 trNHO-1g-N2

23 trNHOvdw-1g-N2

24 trNHOts-1g-N2

25 trNHOadd-1g-N2

26 trNHO-1f-N2

27 trNHOvdw-1f-N2

28 trNHOts-1f-N2

29 trNHOadd-1f-N2

30 trNHO-1c-N2

31 trNHOvdw-1c-N2
32 trNHOTs-1c-N2
33 trNHOadd-1c-N2

34 trNHO-1b-N2
35 trNHOvdw-1b-N2
36 trNHOTs-1b-N2
37 trNHOadd-1b-N2

38 trNHO-1a-N2
39 trNHOvdw-1a-N2
40 trNHOTs-1a-N2
41 trNHOadd-1a-N2

42 trNHO-1k-N2
43 trNHOvdw-1k-N2
44 trNHOTs-1k-N2
45 trNHOadd-1k-N2

46 trNHO-1j-N2
47 trNHOvdw-1j-N2
48 trNHOTs-1j-N2
49 trNHOadd-1j-N2

50 trNHO-1i-N2
51 trNHOvdw-1i-N2
52 trNHOTs-1i-N2
53 trNHOadd-1i-N2

54 trNHO-1e-N4
55 trNHOvdw-1e-N4
56 trNHOTs-1e-N4
57 trNHOadd-1e-N4

58 trNHO-1d-N4
59 trNHOvdw-1d-N4
60 trNHOTs-1d-N4
61 trNHOadd-1d-N4

62 trNHO-1h-N4
63 trNHOvdw-1h-N4
64 trNHOTs-1h-N4
65 trNHOadd-1h-N4

66 trNHO-1g-N4
67 trNHOvdw-1g-N4
68 trNHOTs-1g-N4

69 trNHOadd-1g-N4

70 trNHO-1f-N4

71 trNHOvdw-1f-N4

72 trNHOts-1f-N4

73 trNHOadd-1f-N4

74 trNHO-1c-N4

75 trNHOvdw-1c-N4

76 trNHOts-1c-N4

77 trNHOadd-1c-N4

78 trNHO-1b-N4

79 trNHOvdw-1b-N4

80 trNHOts-1b-N4

81 trNHOadd-1b-N4

82 trNHO-1a-N4

83 trNHOvdw-1a-N4

84 trNHOts-1a-N4

85 trNHOadd-1a-N4

86 trNHO-1k-N4

87 trNHOvdw-1k-N4

88 trNHOts-1k-N4

89 trNHOadd-1k-N4

90 trNHO-1j-N4

91 trNHOvdw-1j-N4

92 trNHOts-1j-N4

93 trNHOadd-1j-N4

94 trNHO-1i-N4

95 trNHOvdw-1i-N4

96 trNHOts-1i-N4

97 trNHOadd-1i-N4

98 trNHO_1e_N2_1e_N4

99 trNHOvdw_1e_N2_1e_N4

100 trNHOts_1e_N2_1e_N4

101 trNHOadd_1e_N2_1e_N4

102 trNHO_1e_N2_1j_N4

103 trNHOvdw_1e_N2_1j_N4

104 trNHOts_1e_N2_1j_N4

105 trNHOadd_1e_N2_1j_N4

106 trNHO_1e_N2_1i_N4
107 trNHOvdw_1e_N2_1i_N4
108 trNHOts_1e_N2_1i_N4
109 trNHOadd_1e_N2_1i_N4

Frames ranges from 1-109
optimized geometries

3

CO2

C -1.4783 7.4522 2.8864

O -1.3451 7.4716 1.7140

O -1.6117 7.4330 4.0587

18

NHO

N -0.3037 1.9471 3.3123

N -2.1274 0.7605 2.9783

C -1.5031 1.5820 3.9038

C -2.0041 2.0130 5.1117

H -1.3691 2.5657 5.7870

H -2.9110 1.5774 5.5023

C -0.2867 1.5145 1.9864

H 0.5565 1.6955 1.3405

C 0.5470 2.9802 3.8654

C -1.4139 0.7799 1.7802

H -1.7278 0.2098 0.9218

C -3.5036 0.3352 3.1264

H -3.6215 -0.2433 4.0426

H -3.7692 -0.2933 2.2798

H -4.1746 1.1979 3.1623

H 0.8793 2.6979 4.8643

H 1.4197 3.0928 3.2268

H 0.0138 3.9331 3.9238

21

NHOvdw

N -0.3057 1.9569 3.3235

O -2.6701 3.8757 2.4734

N -2.1414 0.7897 2.9866

O -3.7746 4.7387 4.3744

C -1.4826 1.5555 3.9355

C -3.2094 4.2839 3.4427

C -1.9452 1.9275 5.1771

H -1.2996 2.4671 5.8526

H -2.8571 1.4997 5.5642

C -0.3222 1.5772 1.9817

H 0.5063 1.7807 1.3234

C 0.5441 2.9803 3.8930
C -1.4570 0.8556 1.7736
H -1.7967 0.3250 0.8996
C -3.5191 0.3789 3.1491
H -3.6262 -0.2424 4.0386
H -3.8169 -0.2025 2.2795
H -4.1768 1.2484 3.2444
H 0.9185 2.6629 4.8665
H 1.3907 3.1424 3.2299
H -0.0063 3.9186 4.0141
21

NHOts

N -0.3366 1.9903 3.2777
O -2.6626 3.9141 2.5753
N -2.1459 0.8062 2.9481
O -3.7503 4.6674 4.5224
C -1.5467 1.6627 3.8412
C -3.1257 4.1371 3.6543
C -2.1480 2.2770 4.9343
H -1.5149 2.8157 5.6262
H -3.0340 1.8186 5.3519
C -0.2226 1.4049 2.0235
H 0.6623 1.5154 1.4195
C 0.5285 3.0194 3.8189
C -1.3509 0.6659 1.8181
H -1.6259 0.0217 0.9999
C -3.5188 0.3639 3.0871
H -3.6444 -0.2121 4.0038
H -3.7724 -0.2637 2.2366
H -4.1907 1.2258 3.1120
H 0.8308 2.7678 4.8351
H 1.4162 3.0912 3.1956
H 0.0108 3.9818 3.8246
21

NHOadd

N -0.3772 2.0379 3.2031
O -2.7919 4.0242 2.6879
N -2.1503 0.8346 2.8665
O -3.6481 4.6520 4.7144
C -1.6352 1.8155 3.6378
C -3.0027 3.9027 3.9309
C -2.3714 2.6382 4.6156
H -1.7096 2.9653 5.4189
H -3.1666 2.0578 5.0845
C -0.0883 1.1862 2.1630
H 0.8700 1.1767 1.6719
C 0.5188 3.0626 3.7413

C -1.2105 0.4249 1.9494
H -1.3978 -0.3646 1.2417
C -3.5179 0.3212 2.9704
H -3.6653 -0.1572 3.9363
H -3.6598 -0.4120 2.1819
H -4.2242 1.1374 2.8373
H 0.8502 2.7846 4.7397
H 1.3795 3.1359 3.0832
H -0.0008 4.0175 3.7598

17

trNHO

N -0.0305 1.1866 3.3626
N -2.0291 0.7809 2.5993
C -1.2986 0.8136 3.7834
C -1.7507 0.5908 5.0547
H -1.0599 0.6098 5.8831
H -2.7407 0.1929 5.2155
N -0.0369 1.6105 2.0387
C 0.9729 1.7271 4.2555
C -1.2459 1.3279 1.6151
H -1.5788 1.4529 0.5972
C -3.4577 0.5382 2.5462
H 1.1980 0.9971 5.0314
H 1.8711 1.9141 3.6730
H 0.6290 2.6561 4.7203
H -3.6782 -0.4698 2.8956
H -3.7918 0.6369 1.5164
H -3.9841 1.2623 3.1709

20

trNHOvdw

N -0.0560 1.2415 3.3637
O -1.8873 3.6696 4.0759
N -2.0704 0.8271 2.6555
O -2.9198 3.4141 6.1844
C -1.2796 0.7585 3.7977
C -2.3991 3.5173 5.1302
C -1.6546 0.3699 5.0542
H -0.9339 0.3611 5.8572
H -2.6289 -0.0621 5.2224
N -0.1364 1.7783 2.0871
C 0.9821 1.7068 4.2562
C -1.3528 1.4872 1.6905
H -1.7436 1.7064 0.7097
C -3.4904 0.5374 2.6452
H 1.2922 0.8942 4.9121
H 1.8288 2.0169 3.6496
H 0.6342 2.5491 4.8620

H -3.6631 -0.5126 2.8798
H -3.8880 0.7511 1.6563
H -4.0053 1.1580 3.3824
20

trNHOts

N -0.0871 1.3373 3.3734
O -1.9511 3.6928 4.2058
N -2.0425 0.8549 2.6049
O -2.9427 3.2674 6.2946
C -1.3361 0.9681 3.7832
C -2.3951 3.2587 5.2307
C -1.8434 0.9652 5.0750
H -1.1355 0.9147 5.8916
H -2.7989 0.4856 5.2394
N 0.0017 1.4936 2.0122
C 1.0026 1.7298 4.2412
C -1.2041 1.1881 1.5769
H -1.4933 1.1673 0.5390
C -3.4640 0.5654 2.5311
H 1.2061 0.9396 4.9630
H 1.8783 1.8852 3.6179
H 0.7517 2.6526 4.7683
H -3.6726 -0.4043 2.9809
H -3.7611 0.5456 1.4859
H -4.0246 1.3422 3.0526

20

trNHOadd

N -0.1016 1.3926 3.3527
O -2.0105 3.6755 4.2999
N -2.0461 0.9168 2.5929
O -2.9069 3.1606 6.3444
C -1.3668 1.1732 3.7335
C -2.3290 2.9070 5.2548
C -1.9373 1.3923 5.0724
H -1.2156 1.1194 5.8436
H -2.8161 0.7654 5.2233
N 0.0587 1.2816 2.0108
C 1.0140 1.8170 4.1959
C -1.1542 0.9828 1.5652
H -1.4019 0.8273 0.5289
C -3.4801 0.6275 2.4974
H 1.1085 1.1443 5.0441
H 1.9079 1.7674 3.5833
H 0.8350 2.8362 4.5311
H -3.6970 -0.3139 2.9966
H -3.7367 0.5476 1.4456
H -4.0410 1.4426 2.9476

26

trNHO-1e-N2

N -0.0308 1.4421 3.3861
N -2.0196 1.0488 2.5931
C -1.3255 1.1464 3.7970
C -1.8854 0.9765 5.0394
H -1.3110 1.0497 5.9448
H -2.9339 0.7335 5.1154
N 0.0673 1.5318 2.0077
C 1.1533 1.7032 4.2337
C -1.1459 1.2877 1.5711
H -1.4269 1.2665 0.5306
C -3.4325 0.7480 2.4945
C 1.4618 0.4479 5.0520
C 2.3450 2.0194 3.3352
C 0.8673 2.9103 5.1293
H -3.6386 -0.2377 2.9137
H -3.7176 0.7589 1.4455
H -4.0131 1.4982 3.0325
H 2.5764 1.1877 2.6715
H 3.2082 2.2033 3.9768
H 2.1650 2.9064 2.7296
H 1.6915 -0.3844 4.3845
H 2.3278 0.6296 5.6909
H 0.6615 3.7888 4.5153
H 1.7384 3.1188 5.7527
H 0.0144 2.7420 5.7838
H 0.6268 0.1581 5.6870

29

trNHOvdw-1e-N2

N -0.0110 1.3119 3.3831
O -2.5481 3.6454 4.0699
N -2.0205 0.9273 2.6290
O -2.9895 3.3400 6.3696
C -1.2607 0.8545 3.7941
C -2.7581 3.4674 5.2188
C -1.7423 0.4394 5.0097
H -1.1407 0.4339 5.9004
H -2.7691 0.1162 5.0854
N -0.0430 1.7738 2.0745
C 1.1448 1.6599 4.2404
C -1.2582 1.5114 1.6573
H -1.6156 1.7066 0.6588
C -3.4313 0.6113 2.5641
C 1.6001 0.4082 4.9932
C 2.2908 2.1296 3.3484
C 0.7446 2.7849 5.1973

H -3.5945 -0.4421 2.7935
H -3.7925 0.8193 1.5599
H -3.9874 1.2227 3.2774
H 2.5651 1.3625 2.6243
H 3.1536 2.3291 3.9859
H 2.0362 3.0402 2.8098
H 1.8738 -0.3745 4.2839
H 2.4756 0.6508 5.5978
H 0.4301 3.6617 4.6285
H 1.5967 3.0642 5.8199
H -0.0673 2.4805 5.8575
H 0.8341 0.0170 5.6580
29

trNHOTs-1e-N2

N -0.0405 1.4381 3.3880
O -2.6372 3.5725 4.1419
N -2.0095 0.9789 2.6088
O -2.9660 3.1712 6.4349
C -1.2973 1.0434 3.7901
C -2.7203 3.1655 5.2644
C -1.8760 0.9402 5.0499
H -1.2492 0.8640 5.9228
H -2.8238 0.4205 5.1064
N 0.0323 1.6117 2.0232
C 1.1538 1.6882 4.2335
C -1.1755 1.3269 1.5871
H -1.4703 1.3487 0.5506
C -3.4204 0.6498 2.5205
C 1.5020 0.4010 4.9819
C 2.3210 2.0754 3.3306
C 0.8501 2.8442 5.1885
H -3.5952 -0.3640 2.8796
H -3.7267 0.7202 1.4801
H -3.9994 1.3554 3.1164
H 2.5562 1.2840 2.6207
H 3.1918 2.2422 3.9662
H 2.1137 2.9896 2.7764
H 1.7305 -0.3946 4.2709
H 2.3804 0.5709 5.6067
H 0.5771 3.7371 4.6235
H 1.7403 3.0673 5.7791
H 0.0427 2.6084 5.8791
H 0.6911 0.0660 5.6256
29

trNHOadd-1e-N2

N -0.0605 1.4694 3.3726
O -2.5880 3.5195 4.2511

N -2.0159 1.0320 2.5880
O -2.9678 3.0127 6.4518
C -1.3368 1.2334 3.7411
C -2.5685 2.7819 5.2792
C -1.9850 1.3360 5.0631
H -1.3058 1.0811 5.8709
H -2.8125 0.6255 5.1169
N 0.0862 1.4046 2.0221
C 1.1408 1.7342 4.2360
C -1.1289 1.1425 1.5653
H -1.3816 1.0338 0.5240
C -3.4560 0.7869 2.4759
C 1.4514 0.4520 5.0057
C 2.3090 2.0905 3.3225
C 0.8373 2.9162 5.1557
H -3.7014 -0.1729 2.9245
H -3.7110 0.7682 1.4204
H -3.9865 1.5981 2.9673
H 2.5560 1.2765 2.6442
H 3.1725 2.2845 3.9593
H 2.1015 2.9859 2.7377
H 1.6568 -0.3660 4.3135
H 2.3357 0.6127 5.6238
H 0.4998 3.7770 4.5782
H 1.7562 3.1882 5.6767
H 0.0901 2.6879 5.9117
H 0.6351 0.1556 5.6631
24

trNHO-1d-N2

N -0.0896 1.1989 3.3297
N -2.1074 1.1288 2.5148
C -1.4203 1.0451 3.7236
C -1.9606 0.8817 4.9662
H -1.3312 0.8089 5.8373
H -3.0272 0.7642 5.0778
N 0.0194 1.5393 1.9840
C 1.0143 1.4176 4.1826
C -1.2121 1.4754 1.5388
H -1.4861 1.6169 0.5056
C -3.5531 1.0943 2.4105
H -3.9292 0.1468 2.7957
H -3.8296 1.1862 1.3633
H -3.9937 1.9169 2.9765
C 2.3876 0.7146 6.0422
C 3.2202 1.8228 5.8463
C 2.9464 2.7245 4.8110
C 1.8395 2.5326 3.9799

C 1.2924 0.4964 5.2017
 H 2.6032 0.0046 6.8323
 H 3.5884 3.5835 4.6541
 H 0.6729 -0.3841 5.3198
 H 1.6076 3.2317 3.1863
 H 4.0747 1.9811 6.4932
 27
 trNHOvdw-1d-N2
 N -0.2795 1.1617 3.2652
 O -1.8614 3.6156 4.1949
 N -2.2426 0.8800 2.3579
 O -1.4163 3.1718 6.4717
 C -1.5605 0.6752 3.5542
 C -1.6365 3.3750 5.3300
 C -2.0796 0.1705 4.7106
 H -1.4723 0.0488 5.5911
 H -3.1112 -0.1446 4.7391
 N -0.2303 1.7783 2.0159
 C 0.7151 1.4860 4.2132
 C -1.4216 1.5733 1.5107
 H -1.7211 1.8795 0.5210
 C -3.6580 0.6165 2.1896
 H -3.8606 -0.4447 2.3334
 H -3.9510 0.9036 1.1826
 H -4.2367 1.1966 2.9112
 C 2.0765 0.8704 6.1142
 C 2.6768 2.1346 6.0974
 C 2.3050 3.0661 5.1207
 C 1.3202 2.7525 4.1802
 C 1.1094 0.5330 5.1632
 H 2.3775 0.1352 6.8515
 H 2.7715 4.0442 5.0963
 H 0.6834 -0.4621 5.1429
 H 1.0171 3.4700 3.4287
 H 3.4308 2.3883 6.8330
 27
 trNHOts-1d-N2
 N -0.1938 1.2265 3.3121
 O -1.8640 3.6045 4.2151
 N -2.1812 0.9954 2.5062
 O -2.7316 3.1874 6.3563
 C -1.4783 0.9229 3.6876
 C -2.2697 3.1484 5.2501
 C -2.0024 0.8634 4.9699
 H -1.3192 0.6770 5.7866
 H -3.0107 0.4900 5.0889
 N -0.0916 1.5452 1.9748

C 0.9003 1.4489 4.1876
C -1.3178 1.3909 1.5203
H -1.6011 1.5108 0.4875
C -3.6265 0.8707 2.4159
H -3.9415 -0.0984 2.7992
H -3.9182 0.9543 1.3722
H -4.1016 1.6667 2.9918
C 2.4553 0.6278 5.8332
C 3.0396 1.8986 5.9019
C 2.5512 2.9423 5.1063
C 1.4689 2.7259 4.2485
C 1.3887 0.3908 4.9615
H 2.8410 -0.1820 6.4411
H 3.0052 3.9249 5.1596
H 0.9432 -0.5933 4.8740
H 1.0656 3.5217 3.6345
H 3.8730 2.0739 6.5717

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trNHOadd-1d-N2

N -0.1942 1.2768 3.2988
O -1.9691 3.6193 4.3508
N -2.1630 1.0645 2.4891
O -2.7736 3.0665 6.4249
C -1.4821 1.1362 3.6527
C -2.2874 2.8292 5.2879
C -2.0412 1.2983 5.0036
H -1.3524 0.9061 5.7512
H -2.9789 0.7512 5.1049
N -0.0249 1.3029 1.9490
C 0.9156 1.4793 4.1812
C -1.2561 1.1682 1.4748
H -1.5125 1.1212 0.4289
C -3.6192 0.9500 2.3600
H -3.9474 -0.0192 2.7278
H -3.8702 1.0439 1.3081
H -4.0883 1.7575 2.9172
C 2.4554 0.6283 5.8093
C 3.0551 1.8913 5.8759
C 2.5791 2.9462 5.0870
C 1.4935 2.7490 4.2294
C 1.3782 0.4072 4.9461
H 2.8311 -0.1857 6.4171
H 3.0466 3.9218 5.1430
H 0.9123 -0.5682 4.8642
H 1.0920 3.5501 3.6215
H 3.8934 2.0538 6.5425

24

trNHO-1h-N2

N -0.1640 1.1320 3.2598
N -2.2112 1.0418 2.5161
C -1.4669 0.8337 3.6744
C -1.9344 0.4430 4.8943
H -1.2634 0.3061 5.7261
H -2.9855 0.2412 5.0294
N -0.1421 1.6779 1.9757
C 0.9250 1.3918 4.1213
C -1.3851 1.5876 1.5706
H -1.7239 1.8709 0.5866
C -3.6555 0.9254 2.4592
H -3.9567 -0.1035 2.6556
H -3.9920 1.2147 1.4669
H -4.1121 1.5844 3.1995
C 2.4222 0.6496 5.8743
C 3.0466 1.8890 5.8008
C 2.6575 2.8864 4.9144
C 1.5739 2.6338 4.0699
C 1.3579 0.3940 5.0056
H 2.7793 -0.1019 6.5668
H 3.1777 3.8359 4.8982
H 0.8788 -0.5770 5.0050
H 1.2263 3.3917 3.3800
F 4.1026 2.1401 6.6440

27

trNHOvdw-1h-N2

N -0.2049 1.1450 3.2488
O -1.7308 3.6414 4.2044
N -2.2306 0.9537 2.4710
O -2.6619 3.2587 6.3412
C -1.4858 0.7342 3.6265
C -2.1929 3.4260 5.2710
C -1.9443 0.2854 4.8296
H -1.2756 0.1668 5.6664
H -2.9833 0.0194 4.9467
N -0.1998 1.7429 1.9906
C 0.8652 1.4096 4.1301
C -1.4293 1.5929 1.5621
H -1.7727 1.9001 0.5869
C -3.6697 0.7910 2.4085
H -3.9386 -0.2507 2.5833
H -4.0148 1.0889 1.4217
H -4.1507 1.4183 3.1623
C 2.4107 0.6403 5.8294
C 2.9788 1.9088 5.8206
C 2.5364 2.9352 4.9942

C 1.4560 2.6815 4.1455
C 1.3514 0.3851 4.9546
H 2.8061 -0.1307 6.4783
H 3.0141 3.9065 5.0252
H 0.9172 -0.6056 4.9028
H 1.0740 3.4580 3.4963
F 4.0335 2.1591 6.6655
27

trNHOts-1h-N2

N -0.2219 1.2245 3.2637
O -1.8092 3.5931 4.2668
N -2.2116 0.9873 2.4659
O -2.7056 3.1221 6.3854
C -1.5037 0.9136 3.6441
C -2.2357 3.1101 5.2816
C -2.0184 0.8420 4.9299
H -1.3308 0.6410 5.7394
H -3.0260 0.4671 5.0505
N -0.1266 1.5486 1.9265
C 0.8748 1.4492 4.1324
C -1.3540 1.3896 1.4777
H -1.6427 1.5111 0.4464
C -3.6547 0.8345 2.3755
H -3.9468 -0.1560 2.7211
H -3.9513 0.9515 1.3366
H -4.1444 1.5977 2.9819
C 2.4374 0.6237 5.7774
C 2.9977 1.8962 5.8044
C 2.5401 2.9524 5.0242
C 1.4498 2.7243 4.1814
C 1.3659 0.3950 4.9108
H 2.8434 -0.1647 6.3982
H 3.0152 3.9234 5.0855
H 0.9198 -0.5896 4.8372
H 1.0480 3.5199 3.5670
F 4.0608 2.1206 6.6422

27

trNHOadd-1h-N2

N -0.2202 1.2687 3.2554
O -1.9268 3.5812 4.3587
N -2.1948 1.0553 2.4612
O -2.7301 3.0185 6.4304
C -1.5033 1.1076 3.6193
C -2.2580 2.7862 5.2871
C -2.0469 1.2529 4.9782
H -1.3601 0.8355 5.7141
H -2.9944 0.7228 5.0787

N -0.0647 1.3298 1.9055
C 0.8921 1.4751 4.1298
C -1.2992 1.1939 1.4408
H -1.5655 1.1716 0.3962
C -3.6513 0.9314 2.3429
H -3.9699 -0.0402 2.7130
H -3.9101 1.0227 1.2928
H -4.1223 1.7358 2.9029
C 2.4478 0.6233 5.7516
C 3.0080 1.8957 5.7909
C 2.5502 2.9639 5.0254
C 1.4618 2.7491 4.1785
C 1.3693 0.4059 4.8910
H 2.8508 -0.1708 6.3668
H 3.0268 3.9330 5.0989
H 0.9141 -0.5746 4.8140
H 1.0532 3.5507 3.5765
F 4.0689 2.1101 6.6285
24

trNHO-1g-N2

N -0.1316 1.1524 3.3162
N -2.1507 1.1379 2.5202
C -1.4617 1.0602 3.7258
C -1.9610 0.9331 4.9868
H -1.2912 0.8688 5.8308
H -3.0235 0.8372 5.1482
N -0.0089 1.4286 1.9540
C 0.9586 1.3759 4.1675
C -1.2459 1.3905 1.5217
H -1.5254 1.5087 0.4870
C -3.5968 1.0991 2.4171
H -3.9718 0.1519 2.8046
H -3.8744 1.1916 1.3704
H -4.0364 1.9228 2.9814
C 2.6434 0.5105 5.7172
C 3.1561 1.8040 5.8629
C 2.5948 2.8898 5.1807
C 1.4984 2.6532 4.3637
C 1.5612 0.3253 4.8682
H 3.0718 -0.3364 6.2375
H 2.9817 3.8949 5.2896
F 1.0550 -0.9271 4.6915
F 0.9120 3.6916 3.7053
H 4.0061 1.9677 6.5129

27

trNHOvdw-1g-N2

N -0.2582 1.3489 3.5193

O -2.2395 3.8416 3.3390
N -2.2299 0.8003 2.8015
O -2.6646 4.2813 5.6196
C -1.5211 0.9851 3.9818
C -2.4409 4.0413 4.4856
C -1.9661 0.8803 5.2655
H -1.2992 1.0857 6.0893
H -2.9929 0.6186 5.4694
N -0.1570 1.2882 2.1300
C 0.9062 1.4000 4.2962
C -1.3725 0.9777 1.7481
H -1.6757 0.8890 0.7172
C -3.6428 0.4830 2.7545
H -3.8346 -0.4559 3.2753
H -3.9444 0.3841 1.7148
H -4.2214 1.2813 3.2225
C 3.0080 0.3890 5.0444
C 3.2578 1.5198 5.8305
C 2.3572 2.5898 5.8691
C 1.2056 2.5065 5.0988
C 1.8301 0.3474 4.3124
H 3.6945 -0.4467 5.0074
H 2.5404 3.4707 6.4703
F 1.5453 -0.7497 3.5568
F 0.3224 3.5453 5.1027
H 4.1687 1.5718 6.4132
27

trNHOts-1g-N2

N -0.1901 1.1886 3.3935
O -2.6704 3.7539 3.8046
N -2.1843 0.9679 2.6150
O -2.3466 3.8537 6.1248
C -1.5008 1.1111 3.7981
C -2.4485 3.5453 4.9681
C -2.0266 1.3316 5.0619
H -1.3419 1.2743 5.8979
H -3.0426 1.0054 5.2453
N -0.0393 1.0911 2.0238
C 0.9252 1.3570 4.2315
C -1.2747 0.9570 1.5909
H -1.5466 0.8574 0.5528
C -3.6302 0.8316 2.5133
H -3.9596 -0.0483 3.0644
H -3.8906 0.7191 1.4645
H -4.1083 1.7244 2.9120
C 2.8699 0.4217 5.3709
C 3.1561 1.6914 5.8862

C 2.3520 2.7987 5.5909
C 1.2625 2.6107 4.7523
C 1.7607 0.2825 4.5502
H 3.4873 -0.4380 5.5970
H 2.5729 3.7842 5.9803
F 1.4445 -0.9366 4.0348
F 0.4698 3.6641 4.4180
H 4.0142 1.8192 6.5335
27

trNHOadd-1g-N2

N -0.1813 1.2211 3.3684
O -2.8141 3.6517 3.9486
N -2.1547 1.0292 2.5700
O -2.3270 3.7267 6.1867
C -1.4844 1.2788 3.7120
C -2.4186 3.1842 5.0556
C -2.0252 1.6545 5.0269
H -1.2942 1.4323 5.8037
H -2.9263 1.0735 5.2385
N 0.0029 0.9328 2.0493
C 0.9332 1.3892 4.2267
C -1.2318 0.8202 1.5836
H -1.4789 0.6082 0.5557
C -3.6159 0.9721 2.4346
H -3.9935 0.1210 2.9965
H -3.8492 0.8487 1.3814
H -4.0222 1.9078 2.8066
C 2.8289 0.4252 5.4027
C 3.1470 1.7014 5.8829
C 2.3825 2.8252 5.5480
C 1.2909 2.6499 4.7096
C 1.7228 0.2927 4.5785
H 3.4135 -0.4469 5.6649
H 2.6313 3.8138 5.9117
F 1.3628 -0.9245 4.0935
F 0.5278 3.7058 4.3346
H 4.0038 1.8231 6.5329

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trNHO-1f-N2

N -0.1306 1.0850 3.3148
N -2.1570 1.1733 2.5333
C -1.4636 1.0648 3.7340
C -1.9572 0.9665 4.9987
H -1.2842 0.8700 5.8374
H -3.0216 0.9235 5.1703
N -0.0079 1.3768 1.9524
C 0.9593 1.3295 4.1611

C -1.2482 1.3975 1.5309
H -1.5295 1.5349 0.4989
C -3.6033 1.2428 2.4460
H -4.0441 0.3287 2.8432
H -3.8847 1.3484 1.4016
H -3.9733 2.1002 3.0101
C 2.6896 0.4879 5.6817
C 3.1247 1.8001 5.8295
C 2.5442 2.8928 5.1937
C 1.4527 2.6220 4.3813
C 1.6052 0.2891 4.8377
H 3.1734 -0.3362 6.1889
H 2.9098 3.8999 5.3446
F 1.1481 -0.9755 4.6477
F 0.8283 3.6499 3.7513
F 4.1931 2.0320 6.6454

27

trNH_Ovdw-1f-N₂

N -0.2222 1.1588 3.3086
O -2.5496 3.6301 4.0142
N -2.2340 0.9277 2.5232
O -1.4588 3.5546 6.1074
C -1.5029 0.7503 3.6920
C -1.9993 3.5751 5.0578
C -1.9395 0.3261 4.9098
H -1.2511 0.2366 5.7362
H -2.9678 0.0287 5.0466
N -0.1961 1.6966 2.0200
C 0.8444 1.3962 4.1813
C -1.4227 1.5227 1.5924
H -1.7627 1.7958 0.6058
C -3.6665 0.7204 2.4426
H -3.9047 -0.3293 2.6148
H -4.0093 1.0083 1.4520
H -4.1725 1.3339 3.1900
C 2.5861 0.5285 5.6786
C 2.9634 1.8445 5.9210
C 2.3453 2.9508 5.3473
C 1.2844 2.6904 4.4922
C 1.5351 0.3414 4.7911
H 3.0999 -0.3082 6.1321
H 2.6598 3.9607 5.5729
F 1.1463 -0.9254 4.4937
F 0.6212 3.7356 3.9308
F 4.0029 2.0661 6.7762

27

trNH_Ots-1f-N₂

N -0.1889 1.1631 3.3818
O -2.6705 3.7531 3.8484
N -2.1824 0.9883 2.5902
O -2.2464 3.8153 6.1532
C -1.5032 1.1015 3.7783
C -2.4034 3.5210 4.9985
C -2.0296 1.3084 5.0444
H -1.3505 1.2168 5.8819
H -3.0536 1.0017 5.2172
N -0.0331 1.0998 2.0098
C 0.9165 1.3490 4.2269
C -1.2680 0.9890 1.5697
H -1.5384 0.9042 0.5296
C -3.6295 0.8697 2.4781
H -3.9740 0.0088 3.0494
H -3.8816 0.7295 1.4307
H -4.1002 1.7785 2.8483
C 2.8543 0.4375 5.4077
C 3.1079 1.7258 5.8677
C 2.3310 2.8376 5.5579
C 1.2532 2.6173 4.7129
C 1.7532 0.2853 4.5779
H 3.4869 -0.3992 5.6725
H 2.5703 3.8249 5.9305
F 1.4509 -0.9449 4.0936
F 0.4703 3.6608 4.3449
F 4.1826 1.9084 6.6845
27

trNHOadd-1f-N2

N -0.1848 1.2137 3.3661
O -2.7740 3.6486 3.9498
N -2.1570 1.0283 2.5642
O -2.2712 3.7184 6.1849
C -1.4884 1.2631 3.7098
C -2.3849 3.1753 5.0564
C -2.0288 1.6352 5.0255
H -1.3085 1.3909 5.8055
H -2.9449 1.0744 5.2258
N 0.0014 0.9490 2.0422
C 0.9254 1.3902 4.2257
C -1.2327 0.8395 1.5745
H -1.4767 0.6485 0.5419
C -3.6184 0.9792 2.4256
H -4.0018 0.1293 2.9847
H -3.8497 0.8588 1.3721
H -4.0206 1.9165 2.7982
C 2.8262 0.4385 5.4156

C 3.1107 1.7264 5.8613
C 2.3670 2.8559 5.5329
C 1.2815 2.6577 4.6930
C 1.7220 0.3023 4.5895
H 3.4293 -0.4142 5.6983
H 2.6327 3.8405 5.8943
F 1.3767 -0.9196 4.1182
F 0.5251 3.7076 4.3046
F 4.1854 1.8904 6.6773

27

trNHO-1c-N2

N -0.1233 1.1152 3.3059
N -2.1602 1.1283 2.5317
C -1.4515 0.9988 3.7234
C -1.9635 0.8368 4.9777
H -1.3077 0.7207 5.8252
H -3.0281 0.7314 5.1179
N -0.0338 1.5079 1.9713
C 0.9774 1.3514 4.1631
C -1.2750 1.4878 1.5495
H -1.5707 1.6804 0.5300
C -3.6083 1.1594 2.4614
H -4.0174 0.2234 2.8406
H -3.9051 1.2797 1.4225
H -3.9982 1.9913 3.0507
C 2.4077 0.6297 5.9704
C 3.1523 1.8160 5.8868
C 2.7880 2.7617 4.9131
C 1.7024 2.5465 4.0623
C 1.3349 0.3837 5.1081
H 2.6785 -0.1223 6.7042
H 3.3503 3.6865 4.8294
H 1.4144 3.2874 3.3264
C 4.3207 2.0742 6.8017
H 4.4738 1.2403 7.4868
H 5.2404 2.2166 6.2315
H 4.1607 2.9746 7.3978
H 0.7880 -0.5506 5.1587

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trNHOvdw-1c-N2

N -0.2721 1.1519 3.2550
O -1.8628 3.6156 4.1668
N -2.2662 0.9192 2.4070
O -1.4266 3.2137 6.4531
C -1.5512 0.6886 3.5788
C -1.6430 3.3953 5.3071
C -2.0388 0.1854 4.7501

H -1.3974 0.0466 5.6040
H -3.0733 -0.1143 4.8156
N -0.2474 1.7808 2.0123
C 0.7618 1.4298 4.1760
C -1.4579 1.6055 1.5413
H -1.7806 1.9265 0.5637
C -3.6939 0.7005 2.2898
H -3.9241 -0.3549 2.4350
H -4.0168 1.0036 1.2970
H -4.2259 1.2928 3.0374
C 2.2221 0.7132 5.9638
C 2.8357 1.9754 6.0043
C 2.3974 2.9530 5.0969
C 1.3656 2.6956 4.1908
C 1.2070 0.4272 5.0478
H 2.5611 -0.0689 6.6352
H 2.8616 3.9340 5.1014
H 1.0321 3.4564 3.4962
C 3.9127 2.2818 7.0113
H 4.4747 1.3834 7.2691
H 4.6135 3.0209 6.6221
H 3.4852 2.6827 7.9332
H 0.7792 -0.5665 4.9956

30

trNHOts-1c-N2

N -0.2012 1.2058 3.2926
O -1.8189 3.6150 4.2394
N -2.1962 1.0042 2.4954
O -2.6040 3.1866 6.4109
C -1.4893 0.9234 3.6741
C -2.1927 3.1565 5.2849
C -2.0058 0.8652 4.9597
H -1.3208 0.6606 5.7703
H -3.0209 0.5116 5.0826
N -0.1006 1.5214 1.9540
C 0.8953 1.4217 4.1660
C -1.3310 1.3851 1.5052
H -1.6174 1.5074 0.4734
C -3.6426 0.8898 2.4084
H -3.9625 -0.0823 2.7805
H -3.9366 0.9874 1.3667
H -4.1109 1.6820 2.9946
C 2.4463 0.5985 5.8143
C 3.0533 1.8624 5.8985
C 2.5554 2.8996 5.0925
C 1.4741 2.6931 4.2326
C 1.3787 0.3652 4.9438

H 2.8250 -0.2192 6.4185
H 3.0125 3.8825 5.1416
H 1.0812 3.4947 3.6192
C 4.1885 2.1102 6.8564
H 4.7644 1.2000 7.0255
H 4.8644 2.8747 6.4724
H 3.8152 2.4527 7.8240
H 0.9321 -0.6189 4.8592
30

trNHOadd-1c-N2

N -0.1969 1.2564 3.2840
O -1.9124 3.6198 4.3678
N -2.1756 1.0746 2.4897
O -2.7038 3.0680 6.4474
C -1.4835 1.1307 3.6476
C -2.2366 2.8292 5.3025
C -2.0258 1.2956 5.0049
H -1.3370 0.8850 5.7425
H -2.9737 0.7675 5.1130
N -0.0389 1.2867 1.9329
C 0.9173 1.4504 4.1612
C -1.2759 1.1708 1.4684
H -1.5415 1.1348 0.4242
C -3.6346 0.9860 2.3734
H -3.9766 0.0227 2.7440
H -3.8929 1.0841 1.3239
H -4.0837 1.8013 2.9355
C 2.4561 0.5999 5.7906
C 3.0720 1.8587 5.8779
C 2.5827 2.9066 5.0793
C 1.5001 2.7169 4.2188
C 1.3799 0.3799 4.9268
H 2.8270 -0.2226 6.3924
H 3.0481 3.8848 5.1345
H 1.1051 3.5241 3.6143
C 4.2114 2.0949 6.8330
H 4.7489 1.1692 7.0391
H 4.9189 2.8172 6.4251
H 3.8448 2.4883 7.7835
H 0.9176 -0.5973 4.8439

30

trNHO-1b-N2

N -0.1115 1.2117 3.3383
N -2.1260 1.1035 2.5389
C -1.4340 1.1029 3.7462
C -1.9391 1.0197 5.0137
H -1.2670 1.0240 5.8581

H -2.9990 0.8978 5.1754
 N 0.0114 1.3879 1.9663
 C 1.0056 1.4090 4.1906
 C -1.2237 1.3033 1.5268
 H -1.5045 1.3594 0.4873
 C -3.5703 1.0333 2.4381
 H -3.9298 0.0982 2.8681
 H -3.8491 1.0738 1.3881
 H -4.0253 1.8734 2.9650
 C 2.6390 0.4933 5.6951
 C 3.1739 1.7732 5.8735
 C 2.6189 2.8696 5.2053
 C 1.5137 2.7106 4.3584
 C 1.5477 0.2856 4.8408
 H 3.0786 -0.3528 6.2126
 H 3.0369 3.8597 5.3543
 C 0.9747 -1.0841 4.6009
 H 0.9219 -1.3022 3.5324
 H 1.5942 -1.8445 5.0768
 H -0.0376 -1.1662 5.0028
 C 0.8913 3.8797 3.6443
 H -0.1978 3.8382 3.6986
 H 1.2177 4.8166 4.0964
 H 1.1660 3.8938 2.5882
 H 4.0227 1.9167 6.5324
 33
 trNHOvdw-1b-N2
 N -0.1320 1.1684 3.3150
 O -3.0203 3.6917 4.2039
 N -2.1271 0.9830 2.4773
 O -1.8774 3.6872 6.2705
 C -1.4424 0.8883 3.6848
 C -2.4437 3.6632 5.2351
 C -1.9489 0.5932 4.9193
 H -1.2978 0.5761 5.7799
 H -3.0030 0.3968 5.0442
 N -0.0184 1.5092 1.9730
 C 0.9475 1.3871 4.2082
 C -1.2389 1.3657 1.5076
 H -1.5122 1.5054 0.4738
 C -3.5490 0.7409 2.3368
 H -3.7840 -0.2829 2.6313
 H -3.8275 0.8876 1.2960
 H -4.1107 1.4360 2.9614
 C 2.5785 0.4864 5.7272
 C 3.0192 1.7846 6.0047
 C 2.4288 2.8803 5.3677

C 1.3688 2.7050 4.4674
 C 1.5430 0.2624 4.8104
 H 3.0531 -0.3605 6.2113
 H 2.7772 3.8841 5.5879
 C 1.0935 -1.1256 4.4446
 H 1.1184 -1.2674 3.3620
 H 1.7453 -1.8692 4.9039
 H 0.0701 -1.3143 4.7764
 C 0.7281 3.8824 3.7834
 H -0.3242 3.6961 3.5716
 H 0.8058 4.7726 4.4088
 H 1.2105 4.0955 2.8270
 H 3.8277 1.9415 6.7097
 33
 trNHOts-1b-N2
 N -0.1353 1.2328 3.3173
 O -2.8804 3.5640 4.1462
 N -2.1264 1.0593 2.5005
 O -2.1257 3.4393 6.3679
 C -1.4414 1.0377 3.6956
 C -2.4505 3.2697 5.2275
 C -1.9711 1.0097 4.9768
 H -1.2826 0.8650 5.7976
 H -2.9777 0.6323 5.1041
 N 0.0028 1.4256 1.9576
 C 0.9624 1.4216 4.2016
 C -1.2250 1.2975 1.4974
 H -1.4944 1.3649 0.4557
 C -3.5585 0.8388 2.3701
 H -3.8131 -0.1600 2.7241
 H -3.8259 0.9267 1.3204
 H -4.0987 1.5889 2.9446
 C 2.5675 0.4964 5.7230
 C 3.0637 1.7832 5.9570
 C 2.5063 2.8863 5.3029
 C 1.4296 2.7298 4.4192
 C 1.5100 0.2880 4.8281
 H 3.0128 -0.3543 6.2277
 H 2.8971 3.8803 5.4932
 C 0.9819 -1.0886 4.5277
 H 0.9265 -1.2607 3.4510
 H 1.6344 -1.8465 4.9613
 H -0.0205 -1.2314 4.9374
 C 0.8237 3.9049 3.7004
 H -0.2539 3.7910 3.5823
 H 1.0112 4.8249 4.2551
 H 1.2493 4.0176 2.7008

H 3.8876 1.9258 6.6469
 33
 trNHOadd-1b-N2
 N -0.1454 1.2924 3.3095
 O -2.7763 3.5026 4.1888
 N -2.1155 1.0819 2.4965
 O -2.2780 3.3230 6.4169
 C -1.4422 1.2138 3.6594
 C -2.3804 2.9061 5.2342
 C -1.9821 1.3969 5.0170
 H -1.2389 1.0939 5.7534
 H -2.8738 0.7811 5.1573
 N 0.0358 1.2151 1.9625
 C 0.9651 1.4620 4.2028
 C -1.1966 1.0848 1.4874
 H -1.4446 0.9868 0.4434
 C -3.5724 0.9762 2.3592
 H -3.9045 0.0064 2.7230
 H -3.8158 1.0739 1.3057
 H -4.0210 1.7905 2.9208
 C 2.5654 0.5039 5.6872
 C 3.0640 1.7862 5.9378
 C 2.5077 2.9035 5.3063
 C 1.4314 2.7672 4.4193
 C 1.4982 0.3107 4.8007
 H 3.0100 -0.3549 6.1776
 H 2.9050 3.8917 5.5088
 C 0.9405 -1.0556 4.5043
 H 0.8009 -1.2051 3.4320
 H 1.6228 -1.8258 4.8628
 H -0.0233 -1.2140 4.9947
 C 0.8204 3.9443 3.7081
 H -0.2685 3.9401 3.7838
 H 1.1841 4.8747 4.1434
 H 1.0821 3.9416 2.6476
 H 3.8915 1.9152 6.6257
 33
 trNHO-1a-N2
 N -0.1145 1.2069 3.3353
 N -2.1295 1.1101 2.5352
 C -1.4374 1.1030 3.7422
 C -1.9438 1.0200 5.0095
 H -1.2720 1.0123 5.8540
 H -3.0044 0.9013 5.1698
 N 0.0095 1.3825 1.9631
 C 1.0025 1.4005 4.1879
 C -1.2261 1.3056 1.5232

H -1.5067 1.3650 0.4838
 C -3.5741 1.0459 2.4341
 H -3.9374 0.1116 2.8626
 H -3.8527 1.0894 1.3842
 H -4.0258 1.8869 2.9626
 C 2.6371 0.4901 5.6937
 C 3.1867 1.7643 5.8891
 C 2.6164 2.8532 5.2110
 C 1.5141 2.6998 4.3631
 C 1.5459 0.2810 4.8392
 H 3.0721 -0.3621 6.2080
 H 3.0314 3.8465 5.3602
 C 0.9764 -1.0912 4.6025
 H 0.9201 -1.3109 3.5343
 H 1.6003 -1.8495 5.0764
 H -0.0341 -1.1771 5.0083
 C 0.8964 3.8738 3.6525
 H -0.1929 3.8391 3.7112
 H 1.2302 4.8085 4.1041
 H 1.1664 3.8878 2.5951
 C 4.3664 1.9735 6.8036
 H 4.6784 1.0351 7.2623
 H 5.2188 2.3819 6.2573
 H 4.1221 2.6752 7.6035
 36
 trNHOvdw-1a-N2
 N -0.1411 1.1700 3.3112
 O -2.9878 3.6963 4.2120
 N -2.1413 0.9824 2.4862
 O -1.8473 3.6800 6.2798
 C -1.4485 0.8883 3.6891
 C -2.4120 3.6614 5.2436
 C -1.9474 0.5942 4.9272
 H -1.2902 0.5754 5.7829
 H -3.0007 0.3979 5.0588
 N -0.0352 1.5036 1.9668
 C 0.9479 1.3826 4.1936
 C -1.2591 1.3614 1.5096
 H -1.5392 1.4990 0.4775
 C -3.5650 0.7456 2.3560
 H -3.8018 -0.2774 2.6514
 H -3.8509 0.8944 1.3176
 H -4.1193 1.4423 2.9854
 C 2.6007 0.4825 5.6880
 C 3.0779 1.7736 5.9594
 C 2.4683 2.8616 5.3197
 C 1.3889 2.6948 4.4423

C 1.5473 0.2595 4.7933
 H 3.0772 -0.3711 6.1621
 H 2.8289 3.8665 5.5215
 C 1.0895 -1.1295 4.4405
 H 1.1030 -1.2778 3.3586
 H 1.7440 -1.8726 4.8968
 H 0.0692 -1.3141 4.7832
 C 0.7519 3.8788 3.7659
 H -0.3039 3.7014 3.5640
 H 0.8419 4.7673 4.3926
 H 1.2267 4.0909 2.8054
 C 4.1983 1.9859 6.9443
 H 4.9065 1.1567 6.9162
 H 4.7433 2.9050 6.7257
 H 3.8157 2.0604 7.9651
 36
 trNHOTs-1a-N2
 N -0.1405 1.2271 3.3083
 O -2.8729 3.5798 4.1653
 N -2.1378 1.0538 2.5057
 O -2.0581 3.4564 6.3651
 C -1.4448 1.0384 3.6962
 C -2.4162 3.2849 5.2352
 C -1.9645 1.0150 4.9807
 H -1.2707 0.8695 5.7967
 H -2.9735 0.6471 5.1163
 N -0.0102 1.4039 1.9454
 C 0.9630 1.4144 4.1851
 C -1.2416 1.2768 1.4943
 H -1.5181 1.3311 0.4539
 C -3.5717 0.8391 2.3869
 H -3.8284 -0.1586 2.7424
 H -3.8479 0.9298 1.3396
 H -4.1033 1.5908 2.9673
 C 2.5864 0.4928 5.6881
 C 3.0992 1.7749 5.9358
 C 2.5184 2.8702 5.2804
 C 1.4333 2.7193 4.4082
 C 1.5207 0.2834 4.8047
 H 3.0374 -0.3646 6.1795
 H 2.9083 3.8672 5.4650
 C 0.9994 -1.0958 4.5027
 H 0.9465 -1.2677 3.4257
 H 1.6543 -1.8513 4.9370
 H -0.0034 -1.2434 4.9100
 C 0.8235 3.9005 3.7023
 H -0.2588 3.8014 3.6177

H 1.0403 4.8201 4.2468
H 1.2183 4.0037 2.6891
C 4.2208 1.9774 6.9210
H 4.8914 1.1176 6.9335
H 4.8058 2.8634 6.6731
H 3.8321 2.1088 7.9338
36
trNHOadd-1a-N2
N -0.1441 1.2793 3.3020
O -2.6034 3.5666 4.2261
N -2.1228 1.1110 2.4996
O -2.4904 3.1978 6.4840
C -1.4392 1.2137 3.6591
C -2.3936 2.8801 5.2701
C -1.9746 1.3828 5.0200
H -1.2220 1.0878 5.7505
H -2.8519 0.7486 5.1675
N 0.0258 1.2181 1.9523
C 0.9738 1.4502 4.1842
C -1.2115 1.1122 1.4839
H -1.4672 1.0272 0.4406
C -3.5821 1.0313 2.3758
H -3.9188 0.0339 2.6501
H -3.8419 1.2346 1.3413
H -4.0165 1.7918 3.0178
C 2.5768 0.5145 5.6797
C 3.1192 1.7893 5.8988
C 2.5611 2.8874 5.2275
C 1.4735 2.7488 4.3571
C 1.4950 0.3119 4.8146
H 3.0094 -0.3432 6.1860
H 2.9803 3.8764 5.3860
C 0.9166 -1.0560 4.5674
H 0.7655 -1.2387 3.5016
H 1.5921 -1.8230 4.9451
H -0.0448 -1.1872 5.0703
C 0.8854 3.9196 3.6161
H -0.2028 3.9429 3.7043
H 1.2779 4.8527 4.0199
H 1.1363 3.8789 2.5536
C 4.2593 1.9807 6.8639
H 4.8959 1.0962 6.8981
H 4.8752 2.8336 6.5779
H 3.8873 2.1624 7.8748
28
trNHO-1k-N2
N -0.1763 1.1109 3.2759

N -2.1744 1.0793 2.4145
 C -1.5130 0.9375 3.6309
 C -2.0648 0.7375 4.8641
 H -1.4296 0.6109 5.7268
 H -3.1246 0.5581 4.9605
 N -0.0410 1.5522 1.9617
 C 0.8780 1.3314 4.1954
 C -1.2617 1.5035 1.4834
 H -1.5179 1.7150 0.4572
 C -3.6180 1.0499 2.2795
 H -3.9991 0.0722 2.5734
 H -3.8750 1.2332 1.2392
 H -4.0712 1.8198 2.9065
 C 2.3630 0.4732 5.8967
 C 2.9464 1.7451 6.0252
 C 2.4956 2.8098 5.2311
 C 1.4498 2.5992 4.3241
 C 1.3445 0.2615 4.9725
 H 2.7369 -0.3393 6.5083
 O 3.9502 1.8397 6.9531
 H 2.9307 3.7965 5.3094
 H 1.0832 3.4181 3.7162
 H 0.9087 -0.7231 4.8486
 C 4.5945 3.1146 7.0933
 H 3.8854 3.8782 7.4155
 H 5.3485 2.9714 7.8618
 H 5.0747 3.4124 6.1600
 31
 trNHOvdw-1k-N2
 N -0.3094 1.1200 3.2004
 O -1.8433 3.5687 4.2549
 N -2.2762 0.9465 2.2760
 O -1.4585 3.0031 6.5155
 C -1.6062 0.6658 3.4633
 C -1.6483 3.2618 5.3795
 C -2.1397 0.1273 4.5982
 H -1.5284 -0.0559 5.4658
 H -3.1795 -0.1602 4.6197
 N -0.2330 1.7909 1.9819
 C 0.6842 1.3693 4.1730
 C -1.4288 1.6507 1.4634
 H -1.7123 2.0071 0.4858
 C -3.6992 0.7394 2.0944
 H -3.9408 -0.3155 2.2238
 H -3.9744 1.0459 1.0882
 H -4.2626 1.3306 2.8192
 C 2.0552 0.5955 6.0088

C 2.6565 1.8616 6.0985
 C 2.2829 2.8771 5.2067
 C 1.2892 2.6290 4.2524
 C 1.0908 0.3411 5.0382
 H 2.3777 -0.1867 6.6861
 O 3.6000 1.9982 7.0836
 H 2.7356 3.8586 5.2443
 H 0.9875 3.4111 3.5672
 H 0.6659 -0.6504 4.9434
 C 4.2472 3.2740 7.1958
 H 3.5255 4.0603 7.4225
 H 4.9436 3.1700 8.0225
 H 4.7961 3.5156 6.2840
 31
 trNHOts-1k-N2
 N -0.2397 1.2201 3.2799
 O -1.9170 3.5572 4.2380
 N -2.1922 1.0114 2.3870
 O -2.8310 3.0476 6.3404
 C -1.5359 0.8963 3.5916
 C -2.3493 3.0594 5.2422
 C -2.1064 0.7790 4.8504
 H -1.4534 0.5563 5.6825
 H -3.1195 0.4049 4.9152
 N -0.0854 1.5860 1.9599
 C 0.8180 1.3966 4.2068
 C -1.2923 1.4461 1.4511
 H -1.5348 1.6042 0.4131
 C -3.6299 0.8641 2.2301
 H -3.9421 -0.1160 2.5870
 H -3.8746 0.9526 1.1752
 H -4.1447 1.6445 2.7923
 C 2.3328 0.4806 5.8431
 C 2.8992 1.7546 6.0225
 C 2.4220 2.8495 5.2860
 C 1.3702 2.6662 4.3813
 C 1.3051 0.2955 4.9238
 H 2.7279 -0.3538 6.4103
 O 3.9126 1.8211 6.9399
 H 2.8420 3.8382 5.4080
 H 0.9798 3.5038 3.8162
 H 0.8833 -0.6890 4.7578
 C 4.5376 3.0990 7.1362
 H 3.8202 3.8303 7.5107
 H 5.3075 2.9287 7.8829
 H 4.9958 3.4541 6.2120
 31

trNHOadd-1k-N2

N -0.2361 1.2671 3.2704
O -2.0478 3.5353 4.3201
N -2.1750 1.0793 2.3837
O -2.8465 2.9416 6.3834
C -1.5333 1.0918 3.5712
C -2.3673 2.7252 5.2394
C -2.1323 1.1999 4.9110
H -1.4691 0.7730 5.6628
H -3.0790 0.6614 4.9636
N -0.0235 1.3769 1.9311
C 0.8349 1.4264 4.2034
C -1.2372 1.2587 1.4092
H -1.4586 1.2872 0.3543
C -3.6232 0.9421 2.1978
H -3.9350 -0.0625 2.4735
H -3.8426 1.1137 1.1486
H -4.1308 1.6891 2.8026
C 2.3315 0.4869 5.8275
C 2.9012 1.7585 6.0164
C 2.4330 2.8622 5.2853
C 1.3867 2.6936 4.3737
C 1.3002 0.3130 4.9105
H 2.7163 -0.3520 6.3948
O 3.9065 1.8156 6.9379
H 2.8565 3.8477 5.4190
H 0.9956 3.5360 3.8161
H 0.8679 -0.6662 4.7386
C 4.5620 3.0816 7.1235
H 3.8630 3.8328 7.4921
H 5.3276 2.8982 7.8713
H 5.0276 3.4153 6.1953
32

trNHO-1j-N2

N 0.0901 1.5179 3.3344
N -1.8786 1.3720 2.4379
C -1.2373 1.2872 3.6704
C -1.7872 1.0789 4.9013
H -1.1475 1.0029 5.7673
H -2.8490 0.9169 5.0073
N 0.2716 1.7557 1.9777
C 1.1846 1.5876 4.2125
C -0.9410 1.6556 1.4805
H -1.1775 1.7689 0.4346
C -3.3062 1.1951 2.2595
H -3.6018 0.1957 2.5811
H -3.5449 1.3183 1.2062

H -3.8507 1.9391 2.8420
C 2.7953 0.4283 5.6237
C 3.4557 1.6483 5.8244
C 2.9937 2.8295 5.2474
C 1.8335 2.8096 4.4629
C 1.6583 0.3969 4.8101
H 3.1772 -0.4694 6.0888
H 3.4912 3.7759 5.4196
O 0.9502 -0.7233 4.4887
C 1.4105 -1.9637 5.0486
H 0.7239 -2.7170 4.6735
H 2.4242 -2.1891 4.7142
H 1.3672 -1.9387 6.1385
O 1.4289 3.9992 3.9142
C 0.0161 4.3018 3.9674
H -0.4846 3.9851 3.0535
H -0.4480 3.8334 4.8361
H -0.0473 5.3845 4.0556
H 4.3438 1.6707 6.4452
35

trNHOvdw-1j-N2

N 0.1313 1.4774 3.3353
O -3.1951 3.7915 4.2840
N -1.8364 1.2610 2.4456
O -3.0551 3.2749 6.5838
C -1.1729 1.1253 3.6623
C -3.1104 3.5123 5.4292
C -1.6975 0.7759 4.8721
H -1.0562 0.6917 5.7359
H -2.7424 0.5191 4.9599
N 0.2787 1.8160 1.9952
C 1.2375 1.5413 4.1987
C -0.9300 1.6642 1.5016
H -1.1816 1.8221 0.4651
C -3.2333 0.9278 2.2484
H -3.4066 -0.1187 2.5036
H -3.4870 1.0910 1.2040
H -3.8627 1.5627 2.8720
C 2.8921 0.3790 5.5566
C 3.5339 1.6047 5.7788
C 3.0438 2.7906 5.2342
C 1.8710 2.7676 4.4703
C 1.7476 0.3445 4.7530
H 3.2974 -0.5231 5.9926
H 3.5259 3.7420 5.4218
O 1.0667 -0.7833 4.4021
C 1.5441 -2.0248 4.9444

H 0.8683 -2.7822 4.5581
 H 2.5610 -2.2318 4.6079
 H 1.4996 -2.0154 6.0345
 O 1.4252 3.9636 3.9649
 C 0.0141 4.2306 4.1157
 H -0.5437 3.8952 3.2437
 H -0.3607 3.7481 5.0196
 H -0.0754 5.3111 4.2107
 H 4.4301 1.6280 6.3877
 35
 trNHOts-lj-N2
 N 0.0791 1.5792 3.3555
 O -3.0651 3.4948 4.2357
 N -1.8581 1.2619 2.4556
 O -2.8048 3.0851 6.5339
 C -1.2118 1.2238 3.6723
 C -2.8172 3.0845 5.3356
 C -1.7810 1.0497 4.9215
 H -1.1090 0.9412 5.7619
 H -2.7243 0.5207 4.9783
 N 0.2496 1.8315 2.0070
 C 1.1883 1.6146 4.2258
 C -0.9485 1.6267 1.4995
 H -1.1890 1.7285 0.4538
 C -3.2502 0.8904 2.2518
 H -3.3978 -0.1552 2.5214
 H -3.4934 1.0301 1.2019
 H -3.8921 1.5261 2.8581
 C 2.7982 0.3942 5.5797
 C 3.4840 1.5966 5.7972
 C 3.0359 2.7985 5.2526
 C 1.8709 2.8170 4.4764
 C 1.6558 0.3980 4.7738
 H 3.1727 -0.5218 6.0143
 H 3.5570 3.7308 5.4318
 O 0.9311 -0.7033 4.4274
 C 1.3716 -1.9644 4.9592
 H 0.6701 -2.6965 4.5704
 H 2.3797 -2.2000 4.6156
 H 1.3318 -1.9599 6.0493
 O 1.4882 4.0225 3.9452
 C 0.0957 4.3787 4.0905
 H -0.4955 4.0125 3.2538
 H -0.2909 3.9923 5.0344
 H 0.0704 5.4662 4.1037
 H 4.3778 1.5890 6.4100
 35

trNHOadd-1j-N2

N 0.0637 1.6079 3.3221
O -2.9412 3.3245 4.3678
N -1.8520 1.3162 2.4117
O -2.6498 2.8059 6.5776
C -1.2274 1.3477 3.6069
C -2.5431 2.6153 5.3375
C -1.8313 1.2637 4.9460
H -1.0639 1.0196 5.6790
H -2.5810 0.4686 4.9719
N 0.2864 1.7385 1.9837
C 1.1536 1.6637 4.2345
C -0.9139 1.5586 1.4493
H -1.1286 1.6008 0.3935
C -3.2809 1.0544 2.2021
H -3.5027 0.0273 2.4845
H -3.4963 1.1970 1.1479
H -3.8431 1.7627 2.8032
C 2.7003 0.4421 5.6401
C 3.4087 1.6355 5.8316
C 2.9978 2.8339 5.2498
C 1.8547 2.8607 4.4429
C 1.5705 0.4494 4.8183
H 3.0438 -0.4691 6.1087
H 3.5415 3.7565 5.4097
O 0.8038 -0.6323 4.5014
C 1.2187 -1.9037 5.0385
H 0.4977 -2.6201 4.6567
H 2.2189 -2.1595 4.6879
H 1.1841 -1.8899 6.1282
O 1.5182 4.0457 3.8470
C 0.1412 4.4768 3.9788
H -0.4799 4.0727 3.1819
H -0.2527 4.1920 4.9541
H 0.1677 5.5605 3.8956
H 4.2904 1.6260 6.4614
36

trNHO-1i-N2

N 0.0613 1.5302 3.3490
N -1.8745 1.3495 2.3884
C -1.2723 1.2791 3.6410
C -1.8586 1.0643 4.8544
H -1.2454 0.9999 5.7403
H -2.9211 0.8892 4.9273
N 0.2847 1.7575 1.9967
C 1.1191 1.6204 4.2674
C -0.9095 1.6391 1.4601

H -1.1151 1.7493 0.4073
 C -3.2927 1.1508 2.1651
 H -3.5838 0.1478 2.4798
 H -3.5005 1.2696 1.1048
 H -3.8662 1.8878 2.7286
 C 2.7047 0.4867 5.7310
 C 3.3336 1.7220 5.9683
 C 2.8658 2.8997 5.3848
 C 1.7391 2.8447 4.5509
 C 1.6104 0.4385 4.8732
 H 3.1092 -0.3957 6.2063
 H 3.3100 3.8666 5.5718
 O 0.9459 -0.6989 4.5210
 C 1.4235 -1.9300 5.0863
 H 0.7704 -2.6998 4.6855
 H 2.4528 -2.1240 4.7809
 H 1.3467 -1.9141 6.1746
 O 1.3430 4.0356 3.9977
 C -0.0763 4.3103 3.9685
 H -0.5156 3.9906 3.0244
 H -0.5813 3.8273 4.8055
 H -0.1646 5.3912 4.0578
 O 4.4089 1.6605 6.8159
 C 5.0886 2.8925 7.0995
 H 4.4226 3.5995 7.5964
 H 5.9003 2.6238 7.7689
 H 5.4967 3.3320 6.1882
 39
 trNHOvdw-1i-N2
 N 0.0932 1.5163 3.4158
 O -3.2982 3.7715 3.9896
 N -1.8394 1.2224 2.4735
 O -3.4828 3.4070 6.3153
 C -1.2093 1.1383 3.7117
 C -3.3753 3.5690 5.1513
 C -1.7599 0.8165 4.9186
 H -1.1339 0.7594 5.7963
 H -2.7988 0.5316 4.9871
 N 0.2759 1.8119 2.0700
 C 1.1763 1.5869 4.3064
 C -0.9134 1.6183 1.5449
 H -1.1408 1.7471 0.4988
 C -3.2124 0.8219 2.2366
 H -3.3478 -0.2248 2.5136
 H -3.4354 0.9477 1.1801
 H -3.8929 1.4419 2.8199
 C 2.8564 0.4244 5.6368

C 3.4612 1.6631 5.9149
C 2.9350 2.8560 5.4187
C 1.7755 2.8114 4.6312
C 1.7317 0.3888 4.8184
H 3.3069 -0.4701 6.0427
H 3.3595 3.8243 5.6410
O 1.0956 -0.7489 4.4182
C 1.6404 -1.9939 4.8831
H 1.0101 -2.7620 4.4447
H 2.6683 -2.1205 4.5398
H 1.5926 -2.0568 5.9713
O 1.3194 4.0188 4.1651
C -0.1082 4.2330 4.2068
H -0.5753 3.9317 3.2713
H -0.5442 3.6882 5.0459
H -0.2396 5.3037 4.3514
O 4.5737 1.5888 6.7117
C 5.2302 2.8241 7.0337
H 4.5685 3.4801 7.6011
H 6.0803 2.5442 7.6485
H 5.5811 3.3267 6.1313

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trNHOTs-li-N2

N 0.0481 1.6023 3.3811
O -3.1716 3.4605 4.0974
N -1.8448 1.2338 2.4080
O -2.9994 3.0989 6.4118
C -1.2471 1.2243 3.6497
C -2.9620 3.0769 5.2144
C -1.8615 1.0507 4.8776
H -1.2209 0.9686 5.7451
H -2.7958 0.5037 4.9041
N 0.2677 1.8398 2.0367
C 1.1172 1.6648 4.2964
C -0.9047 1.6049 1.4840
H -1.1100 1.6987 0.4298
C -3.2163 0.8208 2.1518
H -3.3418 -0.2306 2.4102
H -3.4263 0.9602 1.0948
H -3.8993 1.4324 2.7379
C 2.7122 0.4775 5.7011
C 3.3693 1.6966 5.9450
C 2.9081 2.8928 5.3937
C 1.7724 2.8714 4.5722
C 1.6071 0.4601 4.8568
H 3.1149 -0.4217 6.1454
H 3.3777 3.8476 5.5811

O 0.9254 -0.6606 4.4866
C 1.3896 -1.9106 5.0234
H 0.7216 -2.6618 4.6125
H 2.4132 -2.1130 4.7052
H 1.3211 -1.9135 6.1122
O 1.3930 4.0748 4.0331
C -0.0134 4.3975 4.1004
H -0.5458 4.0301 3.2257
H -0.4451 3.9891 5.0149
H -0.0649 5.4841 4.1261
O 4.4574 1.6023 6.7700
C 5.1700 2.8159 7.0554
H 4.5305 3.5294 7.5771
H 5.9901 2.5199 7.7026
H 5.5672 3.2592 6.1413
39
trNHOadd-1i-N2
N 0.0410 1.6097 3.3160
O -3.0070 3.2854 4.3279
N -1.8427 1.3266 2.3366
O -2.7153 2.7330 6.5297
C -1.2581 1.3396 3.5522
C -2.6088 2.5610 5.2866
C -1.8997 1.2175 4.8712
H -1.1547 0.9419 5.6150
H -2.6563 0.4287 4.8489
N 0.3070 1.7640 1.9877
C 1.0867 1.6948 4.2726
C -0.8740 1.5891 1.4101
H -1.0517 1.6493 0.3485
C -3.2637 1.0683 2.0756
H -3.4888 0.0287 2.3037
H -3.4513 1.2613 1.0239
H -3.8451 1.7462 2.6928
C 2.5961 0.5293 5.7670
C 3.2839 1.7403 5.9663
C 2.8719 2.9238 5.3479
C 1.7676 2.8973 4.4882
C 1.5126 0.5018 4.8972
H 2.9552 -0.3574 6.2695
H 3.3693 3.8710 5.4983
O 0.7826 -0.6036 4.5757
C 1.1896 -1.8498 5.1733
H 0.4910 -2.5879 4.7911
H 2.2049 -2.1063 4.8696
H 1.1144 -1.7980 6.2600
O 1.4418 4.0692 3.8588

C 0.0589 4.4918 3.9510
H -0.5418 4.0655 3.1499
H -0.3547 4.2244 4.9229
H 0.0789 5.5737 3.8441
O 4.3416 1.6568 6.8244
C 5.0777 2.8642 7.0842
H 4.4367 3.6179 7.5429
H 5.8586 2.5756 7.7810
H 5.5268 3.2503 6.1684
26

trNHO-1e-N4

N -0.0836 1.4712 3.3785
N -1.9904 0.9425 2.4495
C -1.3828 1.1098 3.7040
C -1.8778 0.9945 4.9764
H -1.2124 1.1535 5.8111
H -2.8686 0.6323 5.1813
N 0.0698 1.7196 2.0283
C -3.3896 0.5201 2.1884
C -1.0792 1.3640 1.5061
H -1.2699 1.3647 0.4481
C 0.8415 2.0683 4.3156
C -4.3498 1.5418 2.7998
C -3.6261 0.4645 0.6804
C -3.5933 -0.8805 2.7670
H 0.4360 2.9958 4.7311
H 1.7644 2.2754 3.7805
H 1.0485 1.3707 5.1266
H -3.5260 1.4451 0.2141
H -4.6479 0.1241 0.5111
H -2.9559 -0.2425 0.1895
H -4.1772 2.5269 2.3629
H -5.3785 1.2453 2.5891
H -2.9090 -1.5839 2.2898
H -4.6165 -1.2085 2.5774
H -3.4205 -0.9098 3.8403
H -4.2328 1.6207 3.8779

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trNHOvdw-1e-N4

N -0.0945 1.4150 3.4526
O -1.9712 3.7806 4.1743
N -1.9951 0.9261 2.4954
O -3.1681 3.3626 6.1672
C -1.3388 0.8750 3.7345
C -2.5652 3.5454 5.1686
C -1.7623 0.4728 4.9745
H -1.0767 0.5398 5.8056

H -2.7186 0.0118 5.1418
N -0.0215 1.9412 2.1805
C -3.3794 0.4766 2.2042
C -1.1642 1.6050 1.6308
H -1.4059 1.8087 0.6037
C 0.8495 1.8407 4.4590
C -4.3643 1.3149 3.0217
C -3.6711 0.6765 0.7182
C -3.4915 -1.0145 2.5237
H 0.4062 2.5898 5.1223
H 1.7076 2.2669 3.9463
H 1.1747 0.9853 5.0513
H -3.6465 1.7284 0.4318
H -4.6771 0.3068 0.5180
H -2.9791 0.1128 0.0909
H -4.2804 2.3675 2.7458
H -5.3842 0.9871 2.8132
H -2.7785 -1.5793 1.9211
H -4.4983 -1.3619 2.2867
H -3.2984 -1.2276 3.5719
H -4.1913 1.2169 4.0916

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trNHOTs-1e-N4

N -0.1351 1.5285 3.4170
O -1.9335 3.7536 4.3620
N -2.0040 0.9780 2.4663
O -3.2027 3.1449 6.2455
C -1.3837 1.0525 3.7088
C -2.5107 3.2337 5.2735
C -1.8961 0.9469 4.9968
H -1.1726 0.8888 5.8001
H -2.8240 0.4274 5.1681
N 0.0468 1.7840 2.0859
C -3.3849 0.4975 2.1846
C -1.0982 1.4342 1.5383
H -1.2898 1.4890 0.4825
C 0.8787 1.8791 4.3874
C -4.3868 1.4266 2.8714
C -3.6294 0.5354 0.6776
C -3.5068 -0.9472 2.6685
H 0.5119 2.6712 5.0429
H 1.7484 2.2272 3.8375
H 1.1493 1.0067 4.9827
H -3.5765 1.5493 0.2792
H -4.6359 0.1608 0.4911
H -2.9337 -0.1061 0.1354
H -4.2464 2.4529 2.5281

H -5.4001 1.1131 2.6151
H -2.7883 -1.5798 2.1446
H -4.5118 -1.3160 2.4583
H -3.3298 -1.0392 3.7377
H -4.2954 1.4059 3.9549

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trNHOadd-1e-N4

N -0.1394 1.5976 3.3821
O -2.0321 3.6943 4.4630
N -1.9867 1.0042 2.4497
O -3.1757 2.9589 6.3061
C -1.4021 1.2387 3.6573
C -2.4558 2.8271 5.2808
C -1.9965 1.3452 5.0032
H -1.2480 1.0758 5.7516
H -2.8307 0.6649 5.1407
N 0.1224 1.6031 2.0566
C -3.3956 0.5442 2.1846
C -1.0240 1.2330 1.5045
H -1.1655 1.1226 0.4453
C 0.8838 2.0206 4.3370
C -4.3691 1.5446 2.8057
C -3.6150 0.5064 0.6747
C -3.5489 -0.8628 2.7585
H 0.5418 2.9223 4.8388
H 1.7831 2.2209 3.7628
H 1.0722 1.2232 5.0516
H -3.5079 1.4930 0.2226
H -4.6367 0.1717 0.4978
H -2.9522 -0.2026 0.1781
H -4.1572 2.5551 2.4558
H -5.3806 1.2762 2.4981
H -2.8304 -1.5441 2.3009
H -4.5548 -1.2252 2.5429
H -3.4122 -0.8881 3.8381
H -4.3467 1.5410 3.8924

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trNHO-1d-N4

N -0.2048 1.4819 3.4336
N -2.1476 1.1698 2.4997
C -1.5425 1.3031 3.7556
C -2.1318 1.2365 4.9844
H -1.5434 1.3654 5.8795
H -3.2063 1.1753 5.0625
N 0.0434 1.2301 2.0894
C -3.5281 0.9004 2.2874
C -1.1447 1.0756 1.5594

H -1.3397 0.9408 0.5076
C 0.8723 1.2902 4.3826
H 0.7437 1.9750 5.2195
H 1.8053 1.5204 3.8753
H 0.8940 0.2612 4.7534
C -5.8184 1.6564 2.2921
C -6.2303 0.3919 1.8525
C -5.2857 -0.6169 1.6330
C -3.9279 -0.3721 1.8632
C -4.4623 1.9204 2.5015
H -6.5494 2.4393 2.4566
H -5.6040 -1.5962 1.2959
H -4.1251 2.8994 2.8209
H -3.1882 -1.1518 1.7216
H -7.2820 0.1954 1.6809

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trNH0vdw-1d-N4

N -0.0556 1.1668 3.3903
O -1.9501 3.6844 4.0094
N -2.0465 1.0075 2.5151
O -3.3500 3.2881 5.8700
C -1.3505 0.7889 3.7128
C -2.6433 3.4621 4.9409
C -1.8414 0.3781 4.9174
H -1.1837 0.2805 5.7674
H -2.8720 0.0746 5.0105
N 0.0117 1.7917 2.1531
C -3.4546 0.9069 2.3663
C -1.1898 1.6567 1.6501
H -1.4827 1.9638 0.6586
C 0.9412 1.4876 4.3895
H 0.6029 2.3053 5.0339
H 1.8504 1.7787 3.8705
H 1.1446 0.6078 4.9990
C -5.5845 1.9352 1.8748
C -6.2166 0.6988 2.0466
C -5.4605 -0.4346 2.3718
C -4.0753 -0.3383 2.5243
C -4.2015 2.0496 2.0505
H -6.1650 2.8144 1.6217
H -5.9466 -1.3953 2.4937
H -3.7065 3.0074 1.9398
H -3.4758 -1.2134 2.7450
H -7.2896 0.6160 1.9209

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trNH0ts-1d-N4

N -0.1303 1.2815 3.4016

O -1.9194 3.6822 4.1538
 N -2.0660 1.0366 2.4841
 O -3.2014 3.2469 6.0740
 C -1.4267 0.9899 3.7110
 C -2.5086 3.2287 5.0967
 C -2.0216 0.9468 4.9626
 H -1.3816 0.8138 5.8250
 H -3.0196 0.5355 5.0277
 N 0.0504 1.5708 2.0698
 C -3.4739 0.8968 2.3076
 C -1.1420 1.4061 1.5373
 H -1.3741 1.5109 0.4903
 C 0.9207 1.5445 4.3631
 H 0.6889 2.4440 4.9371
 H 1.8440 1.6857 3.8086
 H 1.0280 0.6948 5.0360
 C -5.6230 1.8926 1.8718
 C -6.2195 0.6313 1.9843
 C -5.4357 -0.4978 2.2531
 C -4.0530 -0.3720 2.4116
 C -4.2424 2.0356 2.0438
 H -6.2300 2.7652 1.6623
 H -5.8974 -1.4749 2.3299
 H -3.7652 3.0063 1.9789
 H -3.4268 -1.2351 2.6052
 H -7.2904 0.5270 1.8568
 27
 trNHOadd-1d-N4
 N -0.1396 1.3643 3.3728
 O -2.1148 3.7190 4.2424
 N -2.0544 1.0417 2.4732
 O -3.1265 3.1629 6.2222
 C -1.4374 1.2285 3.6651
 C -2.4881 2.9310 5.1618
 C -2.0940 1.4209 4.9671
 H -1.4320 1.1142 5.7783
 H -2.9905 0.8024 5.0261
 N 0.1039 1.2650 2.0398
 C -3.4756 0.9053 2.2938
 C -1.0912 1.0675 1.5028
 H -1.2909 0.9372 0.4522
 C 0.9487 1.6571 4.3057
 H 0.7299 2.5903 4.8189
 H 1.8509 1.7536 3.7108
 H 1.0569 0.8390 5.0139
 C -5.6182 1.9238 1.9555
 C -6.2044 0.6521 1.9510

C -5.4162 -0.4925 2.1206
C -4.0337 -0.3743 2.2913
C -4.2381 2.0635 2.1292
H -6.2324 2.8063 1.8258
H -5.8730 -1.4746 2.1166
H -3.7581 3.0342 2.1539
H -3.4008 -1.2443 2.4224
H -7.2748 0.5528 1.8168
24

trNHO-1h-N4

N -0.0783 1.2178 3.4076
N -2.0201 0.8097 2.5122
C -1.4140 1.0628 3.7482
C -2.0075 1.1407 4.9740
H -1.4183 1.3376 5.8559
H -3.0651 0.9504 5.0741
N 0.1038 1.2806 2.0312
C -3.4141 0.5948 2.3243
C -1.0735 1.0029 1.5297
H -1.2916 0.9003 0.4789
C 0.8908 1.8662 4.2664
H 0.6103 2.9046 4.4657
H 1.8541 1.8330 3.7645
H 0.9615 1.3232 5.2075
C -5.6610 1.4784 2.1954
C -6.0992 0.1818 1.9483
C -5.2488 -0.9156 1.8815
C -3.8818 -0.7012 2.0795
C -4.2921 1.6842 2.3803
H -6.3678 2.2971 2.2323
H -5.6452 -1.9033 1.6832
H -3.9070 2.6790 2.5694
H -3.1833 -1.5284 2.0458
F -7.4430 -0.0244 1.7613
27

trNHOvdw-1h-N4

N -0.0317 1.1895 3.3788
O -2.0265 3.6632 3.8724
N -1.9925 0.8431 2.4942
O -3.2785 3.3796 5.8551
C -1.3122 0.7785 3.7176
C -2.6482 3.4947 4.8640
C -1.8117 0.4605 4.9462
H -1.1689 0.4720 5.8128
H -2.8260 0.1067 5.0461
N 0.0301 1.6896 2.0853
C -3.3874 0.6373 2.3358

C -1.1525 1.4435 1.5795
H -1.4363 1.6281 0.5554
C 0.9297 1.6582 4.3540
H 0.5439 2.5235 4.9022
H 1.8366 1.9331 3.8220
H 1.1576 0.8580 5.0572
C -5.5865 1.5150 1.8331
C -6.0836 0.2299 2.0130
C -5.2854 -0.8608 2.3417
C -3.9135 -0.6509 2.4952
C -4.2157 1.7208 2.0147
H -6.2546 2.3281 1.5791
H -5.7237 -1.8438 2.4591
H -3.7936 2.7118 1.8980
H -3.2530 -1.4782 2.7242
F -7.4303 0.0243 1.8478

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trNHOts-1h-N4

N -0.0828 1.2975 3.3782
O -2.0341 3.6315 3.9625
N -1.9965 0.8791 2.4787
O -3.2508 3.2565 5.9366
C -1.3611 0.9531 3.7066
C -2.5760 3.2088 4.9475
C -1.9586 0.9593 4.9577
H -1.3158 0.9194 5.8272
H -2.9312 0.4950 5.0494
N 0.0874 1.5032 2.0295
C -3.3926 0.6516 2.3112
C -1.0902 1.2336 1.5085
H -1.3259 1.2548 0.4568
C 0.9484 1.6833 4.3200
H 0.6669 2.6076 4.8289
H 1.8660 1.8323 3.7581
H 1.0959 0.8907 5.0523
C -5.5970 1.5198 1.8444
C -6.0795 0.2258 2.0038
C -5.2702 -0.8640 2.3074
C -3.8991 -0.6444 2.4569
C -4.2263 1.7348 2.0109
H -6.2748 2.3303 1.6092
H -5.7000 -1.8520 2.4127
H -3.8085 2.7291 1.9101
H -3.2286 -1.4665 2.6764
F -7.4246 0.0110 1.8467

27

trNHOadd-1h-N4

N -0.0927 1.3760 3.3462
O -2.2299 3.6276 4.0283
N -1.9831 0.8879 2.4704
O -3.2005 3.1677 6.0530
C -1.3773 1.1657 3.6510
C -2.5476 2.8947 5.0121
C -2.0491 1.4025 4.9376
H -1.3699 1.2088 5.7689
H -2.9003 0.7294 5.0459
N 0.1531 1.2416 2.0166
C -3.3922 0.6598 2.3041
C -1.0264 0.9405 1.4944
H -1.2156 0.7672 0.4485
C 0.9752 1.7887 4.2573
H 0.7190 2.7544 4.6871
H 1.8790 1.8660 3.6624
H 1.1036 1.0399 5.0353
C -5.5900 1.5511 1.9139
C -6.0669 0.2468 1.9923
C -5.2541 -0.8578 2.2243
C -3.8820 -0.6460 2.3793
C -4.2192 1.7623 2.0755
H -6.2706 2.3731 1.7336
H -5.6815 -1.8507 2.2782
H -3.7968 2.7587 2.0441
H -3.2091 -1.4763 2.5574
F -7.4104 0.0386 1.8338
24

trNHO-1g-N4

N -0.0127 1.2871 3.2789
N -2.0202 0.9530 2.5019
C -1.3292 1.1817 3.7036
C -1.8516 1.2906 4.9552
H -1.2099 1.4706 5.8035
H -2.9052 1.1204 5.1185
N 0.0795 1.3761 1.8946
C -3.4170 0.8308 2.4081
C -1.1319 1.1461 1.4602
H -1.4100 1.0682 0.4220
C 1.0320 1.8937 4.0791
H 1.1382 1.3410 5.0111
H 0.8051 2.9410 4.2980
H 1.9593 1.8242 3.5173
C -5.6070 1.7839 1.8731
C -6.2135 0.5922 2.2843
C -5.4510 -0.4854 2.7491
C -4.0720 -0.3407 2.8042

C -4.2260 1.8838 1.9666
H -6.1795 2.6283 1.5124
H -5.9083 -1.4132 3.0677
F -3.6083 3.0404 1.5935
F -3.3034 -1.3740 3.2459
H -7.2906 0.4990 2.2313

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trNHOvdw-1g-N4

N 0.0466 1.1571 3.2022
O -2.7148 3.7163 4.1452
N -2.0076 0.9561 2.4917
O -2.9485 3.3052 6.4588
C -1.2352 0.8872 3.6663
C -2.8190 3.4878 5.2994
C -1.6552 0.6619 4.9399
H -0.9490 0.6654 5.7560
H -2.6807 0.3924 5.1378
N 0.0383 1.6036 1.8859
C -3.4042 0.8287 2.4377
C -1.1929 1.4413 1.4818
H -1.5464 1.6185 0.4794
C 1.1167 1.6017 4.0721
H 1.3107 0.8392 4.8252
H 0.8620 2.5446 4.5658
H 2.0061 1.7325 3.4619
C -5.6111 1.7447 1.8935
C -6.2077 0.5599 2.3376
C -5.4295 -0.4986 2.8178
C -4.0500 -0.3475 2.8404
C -4.2298 1.8567 1.9610
H -6.1910 2.5740 1.5100
H -5.8713 -1.4300 3.1474
F -3.6342 3.0008 1.5231
F -3.2707 -1.3827 3.2593
H -7.2848 0.4597 2.3016

27

trNHOts-1g-N4

N -0.0378 1.3277 3.2664
O -2.6724 3.5561 4.1383
N -2.0342 1.0326 2.5058
O -2.7709 3.1425 6.4466
C -1.3055 1.0493 3.6884
C -2.6203 3.1185 5.2559
C -1.8002 1.0125 4.9817
H -1.0840 0.9370 5.7886
H -2.7543 0.5299 5.1428
N 0.0439 1.5402 1.9114

C -3.4303 0.8632 2.4262
 C -1.1771 1.3429 1.4706
 H -1.4820 1.4035 0.4393
 C 1.0903 1.6191 4.1299
 H 1.2353 0.8015 4.8345
 H 0.9178 2.5497 4.6741
 H 1.9683 1.7140 3.4981
 C -5.6390 1.7268 1.8380
 C -6.2155 0.5400 2.3030
 C -5.4256 -0.4949 2.8156
 C -4.0501 -0.3167 2.8519
 C -4.2605 1.8665 1.9128
 H -6.2326 2.5338 1.4287
 H -5.8568 -1.4247 3.1625
 F -3.6752 3.0026 1.4495
 F -3.2516 -1.3171 3.3168
 H -7.2903 0.4193 2.2603
 27
 trNHOadd-1g-N4
 N -0.0729 1.4445 3.2508
 O -2.5268 3.4841 4.2012
 N -2.0312 1.0406 2.4938
 O -2.9433 2.9429 6.3893
 C -1.3287 1.2135 3.6450
 C -2.5185 2.7371 5.2225
 C -1.8822 1.3107 5.0047
 H -1.1019 1.1375 5.7460
 H -2.6489 0.5510 5.1601
 N 0.0614 1.4263 1.8979
 C -3.4389 0.8767 2.4210
 C -1.1569 1.1752 1.4489
 H -1.4194 1.0822 0.4090
 C 1.0796 1.7578 4.0994
 H 1.2444 0.9479 4.8050
 H 0.8934 2.6952 4.6185
 H 1.9354 1.8543 3.4395
 C -5.6312 1.7606 1.8509
 C -6.2119 0.5845 2.3378
 C -5.4306 -0.4560 2.8534
 C -4.0545 -0.2886 2.8824
 C -4.2509 1.8900 1.9046
 H -6.2236 2.5698 1.4447
 H -5.8717 -1.3725 3.2224
 F -3.6522 3.0042 1.4202
 F -3.2523 -1.2713 3.3776
 H -7.2885 0.4762 2.3100
 24

trNHO-1f-N4

N -0.0267 1.1444 3.3964
N -1.9167 0.9967 2.3263
C -1.3949 1.1356 3.6234
C -2.0861 1.2510 4.7896
H -1.5648 1.3608 5.7275
H -3.1627 1.1701 4.7915
N 0.2764 1.2496 2.0443
C -3.2878 0.9693 2.0260
C -0.8716 1.1304 1.4308
H -1.0020 1.0891 0.3609
C 0.9343 1.6337 4.3639
H 0.7608 2.6886 4.5947
H 1.9264 1.5069 3.9391
H 0.8589 1.0443 5.2763
C -5.3225 2.0897 1.2396
C -6.0104 0.9087 1.4969
C -5.4181 -0.2462 1.9966
C -4.0555 -0.1794 2.2504
C -3.9671 2.0921 1.5378
H -5.8213 2.9672 0.8509
H -5.9856 -1.1480 2.1836
F -3.2488 3.2260 1.3284
F -3.4217 -1.2803 2.7275
F -7.3477 0.8778 1.2342

27

trNHOvdw-1f-N4

N 0.0301 1.0085 3.3177
O -2.8986 3.6719 3.9954
N -1.9062 1.0221 2.3139
O -3.1369 3.2595 6.3083
C -1.3229 0.8422 3.5827
C -3.0054 3.4421 5.1493
C -1.9409 0.6104 4.7718
H -1.3619 0.5126 5.6768
H -3.0029 0.4246 4.8102
N 0.2549 1.4915 2.0355
C -3.2805 0.9794 2.0403
C -0.9128 1.4560 1.4514
H -1.0974 1.6927 0.4164
C 1.0034 1.3023 4.3495
H 0.7681 2.2402 4.8616
H 1.9779 1.3760 3.8743
H 1.0210 0.4884 5.0732
C -5.3272 2.0412 1.1960
C -6.0126 0.8754 1.5186
C -5.4092 -0.2482 2.0710

C -4.0429 -0.1666 2.3020
C -3.9695 2.0663 1.4828
H -5.8264 2.8984 0.7640
H -5.9642 -1.1496 2.2945
F -3.2622 3.1856 1.1824
F -3.3980 -1.2553 2.7933
F -7.3518 0.8256 1.2642
27

trNHOTs-1f-N4

N -0.0446 1.1925 3.3771
O -2.8259 3.5241 3.9737
N -1.9266 1.0992 2.3302
O -3.0423 3.0820 6.2685
C -1.3780 1.0124 3.6039
C -2.8334 3.0708 5.0865
C -2.0542 0.9572 4.8120
H -1.4662 0.7927 5.7046
H -3.0509 0.5375 4.8138
N 0.2523 1.4220 2.0561
C -3.2997 1.0182 2.0335
C -0.9042 1.3498 1.4391
H -1.0517 1.4535 0.3768
C 0.9802 1.2889 4.3985
H 0.8078 2.1657 5.0249
H 1.9363 1.3804 3.8915
H 0.9758 0.3900 5.0141
C -5.3474 2.0410 1.1651
C -6.0185 0.8728 1.5100
C -5.4053 -0.2364 2.0818
C -4.0419 -0.1332 2.3180
C -3.9902 2.0879 1.4506
H -5.8583 2.8830 0.7175
H -5.9523 -1.1384 2.3215
F -3.2883 3.2000 1.1249
F -3.3818 -1.1969 2.8437
F -7.3560 0.8050 1.2575

27

trNHOadd-1f-N4

N -0.0605 1.3118 3.3622
O -2.7888 3.4044 4.0119
N -1.9177 1.1124 2.3233
O -3.2013 2.8853 6.2052
C -1.3762 1.1928 3.5688
C -2.7642 2.6734 5.0441
C -2.1055 1.2557 4.8461
H -1.4350 1.0302 5.6746
H -2.8957 0.5033 4.8655

N 0.2652 1.3042 2.0411
C -3.3041 1.0417 2.0348
C -0.8934 1.1833 1.4174
H -1.0240 1.1278 0.3487
C 0.9986 1.4093 4.3706
H 0.7157 2.1452 5.1180
H 1.8936 1.7357 3.8514
H 1.1588 0.4345 4.8252
C -5.3334 2.0667 1.1607
C -6.0111 0.9092 1.5315
C -5.4081 -0.1952 2.1247
C -4.0458 -0.0944 2.3619
C -3.9741 2.1107 1.4328
H -5.8426 2.9030 0.7007
H -5.9626 -1.0866 2.3853
F -3.2571 3.1967 1.0724
F -3.3855 -1.1375 2.9285
F -7.3469 0.8457 1.2819
27

trNHO-1c-N4

N -0.1500 1.4047 3.4303
N -2.0679 1.0788 2.4510
C -1.4953 1.2286 3.7198
C -2.1167 1.1762 4.9337
H -1.5529 1.3196 5.8423
H -3.1931 1.1174 4.9832
N 0.1328 1.1382 2.0957
C -3.4430 0.8096 2.2070
C -1.0417 0.9766 1.5380
H -1.2100 0.8294 0.4831
C 0.9031 1.2269 4.4083
H 0.7502 1.9190 5.2351
H 1.8478 1.4568 3.9229
H 0.9203 0.2018 4.7897
C -5.7308 1.5674 2.1208
C -6.1566 0.2954 1.7022
C -5.1930 -0.7126 1.5444
C -3.8408 -0.4689 1.8025
C -4.3821 1.8347 2.3643
H -6.4593 2.3625 2.2411
H -5.5005 -1.7017 1.2215
H -3.1038 -1.2570 1.6966
C -7.6171 0.0118 1.4703
H -8.1265 0.8878 1.0674
H -7.7499 -0.8119 0.7686
H -8.1147 -0.2615 2.4033
H -4.0553 2.8230 2.6666

30

trNHOvdw-1c-N4

N -0.0384 1.1121 3.4141
O -1.9509 3.6337 3.9267
N -1.9894 0.8991 2.4663
O -3.2833 3.3180 5.8513
C -1.3426 0.7349 3.6980
C -2.6133 3.4495 4.8885
C -1.8817 0.3620 4.8944
H -1.2608 0.2998 5.7748
H -2.9142 0.0552 4.9532
N 0.0756 1.6846 2.1546
C -3.3861 0.7518 2.2564
C -1.1036 1.5171 1.6094
H -1.3574 1.7788 0.5942
C 0.9138 1.4864 4.4378
H 0.5471 2.3345 5.0248
H 1.8441 1.7548 3.9443
H 1.0917 0.6394 5.0994
C -5.5300 1.7067 1.6880
C -6.1433 0.4498 1.8048
C -5.3444 -0.6528 2.1516
C -3.9714 -0.5149 2.3637
C -4.1613 1.8689 1.9234
H -6.1275 2.5733 1.4245
H -5.7969 -1.6352 2.2395
H -3.3567 -1.3745 2.6040
C -7.6130 0.2766 1.5257
H -8.1593 1.2009 1.7157
H -7.7823 -0.0030 0.4834
H -8.0408 -0.5066 2.1523
H -3.6991 2.8466 1.8495

30

trNHOts-1c-N4

N -0.0904 1.2203 3.4149
O -1.9344 3.6120 4.0542
N -1.9902 0.9306 2.4372
O -3.2696 3.2014 5.9436
C -1.3927 0.9168 3.6856
C -2.5471 3.1722 4.9884
C -2.0289 0.8897 4.9171
H -1.4170 0.7802 5.8029
H -3.0243 0.4689 4.9556
N 0.1328 1.4833 2.0840
C -3.3879 0.7617 2.2140
C -1.0384 1.2908 1.5148
H -1.2374 1.3748 0.4589

C 0.9204 1.5196 4.4083
 H 0.6356 2.4078 4.9763
 H 1.8538 1.6996 3.8827
 H 1.0411 0.6735 5.0837
 C -5.5417 1.7045 1.6908
 C -6.1390 0.4381 1.7963
 C -5.3258 -0.6627 2.1131
 C -3.9517 -0.5134 2.3132
 C -4.1710 1.8775 1.9032
 H -6.1533 2.5680 1.4512
 H -5.7682 -1.6501 2.1935
 H -3.3232 -1.3663 2.5432
 C -7.6119 0.2571 1.5408
 H -8.1685 1.1568 1.8046
 H -7.8020 0.0446 0.4865
 H -8.0106 -0.5733 2.1239
 H -3.7148 2.8587 1.8412
 30
 trNHOadd-1c-N4
 N -0.1001 1.3030 3.3830
 O -2.0839 3.6382 4.1518
 N -1.9790 0.9442 2.4235
 O -3.2461 3.1067 6.0537
 C -1.4040 1.1446 3.6340
 C -2.5269 2.8619 5.0494
 C -2.1098 1.3508 4.9077
 H -1.4731 1.0740 5.7495
 H -2.9992 0.7212 4.9481
 N 0.1877 1.2067 2.0588
 C -3.3890 0.7734 2.1999
 C -0.9861 0.9869 1.4844
 H -1.1514 0.8497 0.4286
 C 0.9519 1.6165 4.3495
 H 0.7010 2.5468 4.8532
 H 1.8712 1.7280 3.7840
 H 1.0515 0.8017 5.0629
 C -5.5424 1.7290 1.7597
 C -6.1258 0.4514 1.7856
 C -5.3026 -0.6608 2.0261
 C -3.9284 -0.5133 2.2289
 C -4.1718 1.9047 1.9654
 H -6.1657 2.5984 1.5810
 H -5.7365 -1.6545 2.0525
 H -3.2897 -1.3699 2.4121
 C -7.5989 0.2733 1.5321
 H -8.1577 1.1594 1.8338
 H -7.7923 0.1013 0.4711

H -7.9901 -0.5812 2.0845
H -3.7176 2.8883 1.9678
30
trNHO-1b-N4
N -0.1488 1.2483 3.4727
N -2.1387 0.9669 2.6315
C -1.4842 1.2064 3.8454
C -2.0479 1.3723 5.0769
H -1.4312 1.5501 5.9442
H -3.1141 1.2514 5.1971
N 0.0043 1.2640 2.0919
C -3.5523 0.8505 2.4875
C -1.2045 1.0652 1.6246
H -1.4477 0.9528 0.5803
C 0.8911 1.8327 4.2937
H 0.6943 2.8913 4.4868
H 1.8326 1.7230 3.7622
H 0.9513 1.2967 5.2397
C -5.6835 1.8357 1.9901
C -6.2992 0.6063 2.2414
C -5.5322 -0.5017 2.6160
C -4.1420 -0.3986 2.7540
C -4.2955 1.9866 2.1200
H -6.2850 2.6938 1.7093
H -6.0167 -1.4525 2.8109
C -3.6231 3.3098 1.8674
H -3.1347 3.3371 0.8908
H -4.3578 4.1149 1.8919
H -2.8666 3.5194 2.6243
C -3.2944 -1.5776 3.1479
H -2.7480 -1.3780 4.0717
H -3.9176 -2.4582 3.3039
H -2.5606 -1.8135 2.3748
H -7.3744 0.5107 2.1428
33
trNHOvdw-1b-N4
N -0.1434 1.2697 3.4490
O -1.1509 4.1877 4.5089
N -2.1284 0.9537 2.6330
O -3.2210 4.0704 5.6397
C -1.4469 1.0694 3.8506
C -2.1857 4.0999 5.0734
C -1.9605 1.0163 5.1168
H -1.3180 1.1593 5.9726
H -3.0157 0.8437 5.2638
N -0.0038 1.3376 2.0798
C -3.5435 0.8359 2.5107

C -1.2185 1.1460 1.6171
H -1.4817 1.1110 0.5724
C 0.9848 1.4567 4.3299
H 0.8701 2.3692 4.9184
H 1.8752 1.5312 3.7116
H 1.0791 0.6023 5.0030
C -5.6905 1.8288 2.0986
C -6.2955 0.5872 2.3079
C -5.5151 -0.5329 2.6136
C -4.1231 -0.4288 2.7262
C -4.3005 1.9824 2.2074
H -6.3011 2.6948 1.8652
H -5.9901 -1.4955 2.7698
C -3.6517 3.3188 1.9613
H -3.4139 3.4582 0.9037
H -4.3241 4.1254 2.2559
H -2.7223 3.4229 2.5182
C -3.2616 -1.6257 3.0241
H -2.6929 -1.4825 3.9446
H -3.8780 -2.5175 3.1376
H -2.5468 -1.8061 2.2186
H -7.3721 0.4905 2.2261

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trNHOTs-1b-N4

N -0.1608 1.3368 3.4479
O -1.1657 4.0473 4.4947
N -2.1293 1.0182 2.6191
O -3.1830 3.8993 5.6912
C -1.4667 1.2055 3.8232
C -2.1630 3.7394 5.0853
C -2.0266 1.3999 5.0757
H -1.3779 1.3262 5.9394
H -3.0612 1.1142 5.2068
N 0.0183 1.2410 2.0890
C -3.5463 0.8752 2.4997
C -1.1954 1.0553 1.6120
H -1.4335 0.9363 0.5680
C 0.9704 1.5022 4.3394
H 0.8542 2.4159 4.9213
H 1.8607 1.5709 3.7212
H 1.0520 0.6440 5.0075
C -5.7023 1.8334 2.0817
C -6.2891 0.5873 2.3155
C -5.4942 -0.5168 2.6408
C -4.1033 -0.3929 2.7473
C -4.3140 2.0080 2.1794
H -6.3259 2.6864 1.8357

H -5.9567 -1.4811 2.8212
C -3.6790 3.3448 1.9025
H -3.4077 3.4442 0.8484
H -4.3749 4.1494 2.1417
H -2.7737 3.4931 2.4889
C -3.2271 -1.5671 3.0915
H -2.6806 -1.3950 4.0208
H -3.8316 -2.4653 3.2169
H -2.4932 -1.7601 2.3065
H -7.3646 0.4756 2.2406

33

trNHOadd-1b-N4

N -0.1612 1.3645 3.4263
O -1.2927 3.9413 4.4711
N -2.1173 1.0568 2.6026
O -3.1240 3.7450 5.8322
C -1.4586 1.3504 3.7550
C -2.1833 3.3132 5.1170
C -2.0742 1.7400 5.0341
H -1.4625 1.3943 5.8709
H -3.0616 1.2887 5.1242
N 0.0423 1.0917 2.1124
C -3.5469 0.9124 2.4866
C -1.1757 0.9059 1.6216
H -1.3871 0.6781 0.5897
C 0.9711 1.6635 4.3040
H 0.7812 2.6192 4.7828
H 1.8505 1.7170 3.6704
H 1.0861 0.8665 5.0355
C -5.6909 1.8630 2.0570
C -6.2762 0.6228 2.3256
C -5.4828 -0.4743 2.6739
C -4.0907 -0.3519 2.7688
C -4.3025 2.0428 2.1390
H -6.3161 2.7096 1.7955
H -5.9458 -1.4317 2.8858
C -3.6609 3.3698 1.8320
H -3.2381 3.3817 0.8242
H -4.4066 4.1629 1.8857
H -2.8643 3.6139 2.5355
C -3.2173 -1.5143 3.1595
H -2.6803 -1.3207 4.0909
H -3.8250 -2.4058 3.3102
H -2.4775 -1.7417 2.3894
H -7.3525 0.5121 2.2645

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trNHO-1a-N4

N -0.1287 1.2494 3.4267
N -2.1865 1.0106 2.7505
C -1.4290 1.2134 3.9099
C -1.8857 1.3572 5.1875
H -1.1972 1.5073 6.0047
H -2.9393 1.2402 5.3937
N -0.0932 1.3011 2.0383
C -3.6069 0.9007 2.7202
C -1.3396 1.1256 1.6714
H -1.6723 1.0434 0.6489
C 0.9814 1.8103 4.1684
H 0.8257 2.8740 4.3707
H 1.8807 1.6755 3.5734
H 1.0935 1.2742 5.1094
C -5.7712 1.8847 2.3918
C -6.3887 0.6615 2.6813
C -5.5785 -0.4423 2.9892
C -4.1833 -0.3454 3.0282
C -4.3772 2.0354 2.4165
H -6.3864 2.7487 2.1572
H -6.0455 -1.3969 3.2152
C -3.7328 3.3611 2.1077
H -3.3919 3.4148 1.0711
H -4.4466 4.1707 2.2624
H -2.8716 3.5429 2.7511
C -3.3176 -1.5328 3.3522
H -2.7523 -1.3689 4.2720
H -3.9301 -2.4248 3.4837
H -2.5982 -1.7279 2.5546
C -7.8895 0.5279 2.6836
H -8.3600 1.3820 2.1959
H -8.2022 -0.3766 2.1596
H -8.2769 0.4695 3.7031

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trNHOvdw-1a-N4

N -0.1197 1.2578 3.4077
O -0.9904 4.1843 4.5637
N -2.1737 1.0005 2.7578
O -2.9868 4.0768 5.8206
C -1.3897 1.0802 3.9152
C -1.9889 4.1018 5.1907
C -1.7947 1.0188 5.2196
H -1.0794 1.1385 6.0190
H -2.8365 0.8619 5.4535
N -0.0970 1.3648 2.0336
C -3.5941 0.8922 2.7460
C -1.3500 1.2025 1.6731

H -1.7018 1.1977 0.6538
C 1.0774 1.4370 4.1940
H 1.0250 2.3573 4.7794
H 1.9179 1.4884 3.5073
H 1.2103 0.5880 4.8670
C -5.7645 1.8891 2.4993
C -6.3784 0.6551 2.7479
C -5.5635 -0.4608 2.9910
C -4.1673 -0.3673 3.0018
C -4.3703 2.0394 2.5061
H -6.3832 2.7631 2.3158
H -6.0260 -1.4247 3.1837
C -3.7428 3.3782 2.2187
H -3.6052 3.5330 1.1456
H -4.3810 4.1821 2.5874
H -2.7646 3.4723 2.6871
C -3.2985 -1.5743 3.2311
H -2.6857 -1.4566 4.1267
H -3.9130 -2.4663 3.3517
H -2.6228 -1.7376 2.3891
C -7.8782 0.5164 2.7148
H -8.3639 1.4643 2.9481
H -8.2226 0.1994 1.7277
H -8.2179 -0.2260 3.4379

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trNHOTs-1a-N4

N -0.1428 1.3330 3.4135
O -1.0197 4.0445 4.5220
N -2.1768 1.0641 2.7398
O -2.9127 3.9325 5.9097
C -1.4170 1.2187 3.8898
C -1.9598 3.7536 5.2075
C -1.8724 1.4084 5.1844
H -1.1604 1.3150 5.9945
H -2.9002 1.1446 5.3924
N -0.0744 1.2627 2.0430
C -3.5991 0.9302 2.7288
C -1.3258 1.1048 1.6624
H -1.6500 1.0128 0.6388
C 1.0566 1.4722 4.2155
H 1.0055 2.3869 4.8053
H 1.8996 1.5216 3.5323
H 1.1692 0.6112 4.8753
C -5.7788 1.8936 2.4820
C -6.3726 0.6531 2.7478
C -5.5416 -0.4474 3.0058
C -4.1469 -0.3339 3.0102

C -4.3873 2.0648 2.4773
H -6.4113 2.7556 2.2898
H -5.9897 -1.4140 3.2173
C -3.7745 3.4053 2.1678
H -3.5901 3.5208 1.0966
H -4.4467 4.2071 2.4753
H -2.8240 3.5441 2.6805
C -3.2595 -1.5178 3.2868
H -2.6883 -1.3799 4.2073
H -3.8583 -2.4222 3.3938
H -2.5458 -1.6787 2.4763
C -7.8703 0.4931 2.7210
H -8.3682 1.4287 2.9776
H -8.2153 0.1933 1.7288
H -8.1946 -0.2700 3.4294

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trNHOadd-1a-N4

N -0.1491 1.4127 3.3589
O -1.3579 3.9741 4.4483
N -2.1681 1.0874 2.7198
O -2.6272 3.6777 6.3303
C -1.4101 1.3793 3.8072
C -1.9762 3.2985 5.3228
C -1.8987 1.7334 5.1492
H -1.2289 1.3435 5.9185
H -2.8842 1.2968 5.3116
N -0.0638 1.1509 2.0291
C -3.6021 0.9521 2.7141
C -1.3203 0.9521 1.6542
H -1.6488 0.6939 0.6597
C 1.0481 1.7419 4.1330
H 0.8960 2.7137 4.5948
H 1.8771 1.7734 3.4334
H 1.2201 0.9718 4.8819
C -5.7639 1.9025 2.3860
C -6.3612 0.6796 2.7210
C -5.5367 -0.4048 3.0527
C -4.1411 -0.2967 3.0601
C -4.3733 2.0741 2.3761
H -6.3938 2.7501 2.1338
H -5.9883 -1.3565 3.3159
C -3.7443 3.3886 1.9964
H -3.3294 3.3554 0.9858
H -4.4964 4.1773 2.0155
H -2.9433 3.6687 2.6824
C -3.2595 -1.4620 3.4236
H -2.6987 -1.2757 4.3425

H -3.8639 -2.3543 3.5830
 H -2.5396 -1.6842 2.6336
 C -7.8584 0.5213 2.6890
 H -8.3561 1.4690 2.8958
 H -8.1928 0.1756 1.7083
 H -8.1905 -0.2067 3.4296
 28
 trNHO-1k-N4
 N 0.0809 1.3975 3.4453
 N -1.5778 1.3946 2.0350
 C -1.2905 1.2009 3.3907
 C -2.1655 0.9141 4.3991
 H -1.8109 0.7710 5.4079
 H -3.2083 0.7523 4.1733
 N 0.5820 1.9012 2.2498
 C -2.8732 1.2808 1.4554
 C -0.4339 1.8554 1.4238
 H -0.3921 2.1134 0.3778
 C 0.7943 1.6842 4.6722
 H 0.6604 0.8595 5.3709
 H 0.4353 2.6104 5.1308
 H 1.8496 1.7768 4.4301
 C -4.4774 0.0010 0.1682
 C -5.4033 1.0450 0.3066
 C -5.0572 2.2078 1.0166
 C -3.7939 2.3302 1.5864
 C -3.2100 0.1253 0.7496
 H -4.7184 -0.9013 -0.3762
 H -5.7864 3.0047 1.1007
 H -2.4873 -0.6778 0.6617
 H -3.5176 3.2284 2.1263
 O -6.6704 1.0298 -0.2112
 C -7.0546 -0.1275 -0.9694
 H -8.0722 0.0679 -1.2937
 H -6.4098 -0.2533 -1.8402
 H -7.0336 -1.0246 -0.3491
 31
 trNHOvdw-1k-N4
 N 0.1363 1.3872 3.4396
 O -1.8970 3.5988 4.2526
 N -1.5375 1.4291 2.0472
 O -3.8143 2.8292 5.3975
 C -1.1605 0.9203 3.2962
 C -2.8499 3.1893 4.8200
 C -1.9176 0.2088 4.1811
 H -1.4991 -0.1036 5.1257
 H -2.9024 -0.1302 3.8995

N 0.4734 2.3044 2.4539
C -2.8378 1.3179 1.4876
C -0.5417 2.2832 1.6255
H -0.5907 2.8264 0.6949
C 0.8181 1.4457 4.7144
H 0.9270 0.4394 5.1175
H 0.2647 2.0642 5.4278
H 1.8042 1.8699 4.5454
C -4.5690 -0.0472 0.4838
C -5.3822 1.0900 0.3617
C -4.9160 2.3402 0.8005
C -3.6536 2.4538 1.3771
C -3.2921 0.0755 1.0412
H -4.9001 -1.0183 0.1435
H -5.5603 3.2050 0.6974
H -2.6470 -0.7914 1.1206
H -3.2966 3.4175 1.7222
O -6.6415 1.0877 -0.1748
C -7.1435 -0.1648 -0.6659
H -8.1375 0.0545 -1.0438
H -6.5189 -0.5429 -1.4762
H -7.2119 -0.9006 0.1364

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trNH0ts-1k-N4

N 0.0796 1.4934 3.4505
O -1.9837 3.5963 4.3326
N -1.5420 1.4459 2.0306
O -3.7368 2.6687 5.5924
C -1.2244 1.1103 3.3353
C -2.7884 2.9116 4.9025
C -2.1031 0.7408 4.3418
H -1.6853 0.4017 5.2808
H -3.0502 0.3125 4.0428
N 0.5647 2.0950 2.3131
C -2.8419 1.3228 1.4589
C -0.4416 2.0431 1.4664
H -0.4177 2.3917 0.4463
C 0.8412 1.5115 4.6824
H 0.8702 0.5123 5.1158
H 0.3909 2.2084 5.3925
H 1.8505 1.8310 4.4395
C -4.5504 -0.0439 0.4300
C -5.3773 1.0858 0.3339
C -4.9288 2.3332 0.8006
C -3.6641 2.4542 1.3689
C -3.2756 0.0821 0.9924
H -4.8707 -1.0114 0.0698

H -5.5845 3.1911 0.7148
H -2.6212 -0.7788 1.0638
H -3.3143 3.4119 1.7362
O -6.6370 1.0789 -0.1984
C -7.1239 -0.1670 -0.7217
H -8.1224 0.0488 -1.0892
H -6.4973 -0.5126 -1.5448
H -7.1781 -0.9255 0.0603
31

trNHOadd-1k-N4

N 0.0462 1.5757 3.4389
O -2.0924 3.6399 4.3284
N -1.5694 1.3909 2.0472
O -3.5510 2.7068 5.8275
C -1.2686 1.3383 3.3686
C -2.6712 2.6842 4.9277
C -2.2167 1.2424 4.4895
H -1.7522 0.7440 5.3418
H -3.0873 0.6541 4.1977
N 0.6052 1.7728 2.2166
C -2.8818 1.2659 1.4788
C -0.4092 1.6555 1.3729
H -0.3511 1.7551 0.3014
C 0.8463 1.7344 4.6531
H 0.8131 0.8168 5.2360
H 0.4490 2.5715 5.2220
H 1.8648 1.9366 4.3379
C -4.4682 0.0170 0.1654
C -5.3960 1.0564 0.3332
C -5.0567 2.1975 1.0824
C -3.7948 2.3123 1.6549
C -3.2005 0.1244 0.7475
H -4.7085 -0.8711 -0.4018
H -5.7899 2.9871 1.1925
H -2.4788 -0.6772 0.6416
H -3.5095 3.1904 2.2223
O -6.6571 1.0559 -0.1888
C -7.0328 -0.0649 -1.0064
H -8.0490 0.1439 -1.3255
H -6.3824 -0.1419 -1.8786
H -7.0131 -0.9915 -0.4315

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trNHO-1j-N4

N 0.1271 1.6321 3.3260
N -1.6117 1.3704 2.0428
C -1.2300 1.3519 3.3915
C -2.0084 1.0761 4.4753

H -1.5892 1.0845 5.4697
H -3.0726 0.9479 4.3490
N 0.6022 1.6185 2.0216
C -2.9046 1.0834 1.5572
C -0.4704 1.4955 1.2794
H -0.4828 1.5083 0.2016
C 1.0472 1.3811 4.4141
H 1.0852 0.3168 4.6651
H 0.7335 1.9483 5.2898
H 2.0312 1.7231 4.1042
C -4.4261 -0.3540 0.3308
C -5.4377 0.5884 0.5148
C -5.2080 1.7783 1.2177
C -3.9359 2.0297 1.7436
C -3.1606 -0.1205 0.8799
H -4.6061 -1.2803 -0.2007
H -6.0145 2.4868 1.3444
O -2.1739 -1.0551 0.6583
C -1.5395 -1.6008 1.8405
H -0.6447 -1.0366 2.1013
H -2.2344 -1.6083 2.6804
H -1.2591 -2.6199 1.5827
O -3.5681 3.1591 2.4128
C -4.5823 4.1589 2.6064
H -5.4016 3.7691 3.2119
H -4.0867 4.9652 3.1387
H -4.9555 4.5248 1.6490
H -6.4225 0.4021 0.1031

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trNHOvdw-lj-N4

N 0.0771 1.5042 3.3959
O -1.4011 3.9388 4.6320
N -1.6253 1.2517 2.0788
O -3.4418 3.3430 5.6594
C -1.2416 1.1014 3.4161
C -2.4209 3.6035 5.1248
C -1.9891 0.6385 4.4607
H -1.5637 0.5717 5.4508
H -3.0374 0.4253 4.3166
N 0.5317 1.7951 2.1269
C -2.9184 0.9985 1.5730
C -0.5240 1.6593 1.3583
H -0.5430 1.8404 0.2960
C 0.9934 1.3786 4.5036
H 1.1474 0.3289 4.7683
H 0.5992 1.9140 5.3682
H 1.9383 1.8256 4.2063

C -4.4537 -0.3526 0.2712
 C -5.4555 0.5877 0.5059
 C -5.2130 1.7406 1.2644
 C -3.9392 1.9469 1.8034
 C -3.1812 -0.1604 0.8236
 H -4.6414 -1.2453 -0.3122
 H -6.0118 2.4498 1.4288
 O -2.2111 -1.0818 0.5117
 C -1.4219 -1.6155 1.6020
 H -0.4929 -1.0589 1.7201
 H -1.9879 -1.6006 2.5331
 H -1.1934 -2.6422 1.3233
 O -3.5576 3.0475 2.5187
 C -4.4941 4.1381 2.5579
 H -5.3735 3.8817 3.1500
 H -3.9629 4.9602 3.0297
 H -4.7857 4.4304 1.5483
 H -6.4425 0.4303 0.0873
 35
 trNHOTs-lj-N4
 N 0.1061 1.5218 3.3402
 O -1.4286 3.7739 4.7382
 N -1.6055 1.2897 2.0481
 O -3.5132 3.1039 5.5841
 C -1.2232 1.2140 3.3801
 C -2.4307 3.2085 5.0781
 C -2.0247 1.0162 4.4897
 H -1.5480 0.7310 5.4190
 H -3.0334 0.6645 4.3218
 N 0.5674 1.7490 2.0660
 C -2.9089 1.0338 1.5601
 C -0.4963 1.6129 1.3029
 H -0.5074 1.7283 0.2315
 C 1.0100 1.5293 4.4731
 H 1.1528 0.5180 4.8567
 H 0.6041 2.1695 5.2551
 H 1.9593 1.9304 4.1298
 C -4.4658 -0.3547 0.3346
 C -5.4550 0.6072 0.5399
 C -5.1946 1.7869 1.2491
 C -3.9114 2.0058 1.7620
 C -3.1876 -0.1543 0.8674
 H -4.6708 -1.2694 -0.2076
 H -5.9836 2.5120 1.3903
 O -2.2220 -1.0973 0.6031
 C -1.5157 -1.6465 1.7418
 H -0.5997 -1.0912 1.9403

H -2.1546 -1.6507 2.6252
H -1.2622 -2.6680 1.4667
O -3.5022 3.1228 2.4275
C -4.4655 4.1802 2.5734
H -5.3079 3.8599 3.1869
H -3.9329 4.9838 3.0730
H -4.8105 4.5226 1.5969
H -6.4476 0.4429 0.1380
35

trNHOadd-1j-N4

N 0.1795 1.7932 3.3080
O -1.6089 3.6931 5.0452
N -1.4911 1.3516 2.0422
O -3.7260 2.8645 5.3224
C -1.1255 1.4996 3.3433
C -2.5105 2.8060 4.9957
C -2.0184 1.3924 4.5079
H -1.4860 0.9221 5.3385
H -2.8686 0.7632 4.2467
N 0.6681 1.8300 2.0391
C -2.8187 1.0708 1.6082
C -0.3792 1.5602 1.2745
H -0.3645 1.5134 0.1986
C 1.0698 2.0148 4.4478
H 1.4147 1.0548 4.8276
H 0.5110 2.5676 5.1965
H 1.9079 2.6041 4.0896
C -4.4544 -0.4913 0.7789
C -5.4154 0.5183 0.9006
C -5.1044 1.8003 1.3635
C -3.7820 2.0850 1.7260
C -3.1338 -0.2184 1.1555
H -4.7458 -1.4678 0.4197
H -5.8793 2.5500 1.4397
O -2.0930 -1.0987 1.1339
C -2.3835 -2.4383 0.6913
H -3.1272 -2.9045 1.3380
H -2.7215 -2.4364 -0.3451
H -1.4414 -2.9719 0.7706
O -3.3067 3.2720 2.1821
C -4.2768 4.2901 2.4929
H -4.9876 3.9215 3.2305
H -3.6990 5.1047 2.9168
H -4.7815 4.6266 1.5860
H -6.4374 0.2978 0.6162

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trNHO-1i-N4

N 0.1254 1.5757 3.3589
N -1.5846 1.3699 2.0284
C -1.2392 1.3295 3.3861
C -2.0536 1.0630 4.4458
H -1.6634 1.0528 5.4519
H -3.1164 0.9619 4.2854
N 0.6340 1.5723 2.0672
C -2.8709 1.1323 1.5022
C -0.4225 1.4866 1.2967
H -0.4096 1.5137 0.2190
C 1.0099 1.2966 4.4693
H 1.0003 0.2331 4.7259
H 2.0133 1.5982 4.1806
C -4.4076 -0.2372 0.2001
C -5.3828 0.7516 0.3437
C -5.1276 1.9303 1.0663
C -3.8744 2.1184 1.6430
C -3.1596 -0.0495 0.8094
H -4.5813 -1.1632 -0.3285
H -5.9169 2.6644 1.1464
O -2.2196 -1.0361 0.6148
C -1.5982 -1.5741 1.8071
H -0.6599 -1.0645 2.0228
H -2.2709 -1.4951 2.6613
H -1.3964 -2.6208 1.5891
O -3.4905 3.2303 2.3318
C -4.4666 4.2741 2.4780
H -5.3343 3.9200 3.0365
H -3.9647 5.0553 3.0411
H -4.7716 4.6600 1.5042
O -6.6428 0.6691 -0.1866
C -6.9527 -0.5021 -0.9572
H -7.9781 -0.3642 -1.2875
H -6.2959 -0.5816 -1.8245
H -6.8838 -1.4016 -0.3441
H 0.6985 1.8796 5.3356

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trNHOvdw-1i-N4

N 0.0421 1.3999 3.4602
O -1.3810 3.9020 4.5788
N -1.6304 1.2606 2.0909
O -3.4428 3.3732 5.6008
C -1.2911 1.0525 3.4324
C -2.4130 3.6012 5.0690
C -2.0863 0.5910 4.4426
H -1.6936 0.4789 5.4420
H -3.1374 0.4257 4.2605

N 0.5371 1.7470 2.2217
C -2.9060 1.0409 1.5305
C -0.4999 1.6711 1.4196
H -0.4872 1.8998 0.3664
C 0.9093 1.2658 4.6051
H 1.0124 0.2169 4.8949
H 0.5041 1.8325 5.4451
H 1.8815 1.6692 4.3347
C -4.4082 -0.2457 0.1106
C -5.3996 0.7141 0.3177
C -5.1692 1.8409 1.1264
C -3.9223 2.0060 1.7215
C -3.1630 -0.0823 0.7348
H -4.5582 -1.1247 -0.4992
H -5.9692 2.5574 1.2478
O -2.2082 -1.0243 0.4362
C -1.4522 -1.5846 1.5364
H -0.5165 -1.0459 1.6816
H -2.0380 -1.5716 2.4551
H -1.2351 -2.6111 1.2481
O -3.5574 3.0881 2.4725
C -4.4772 4.1930 2.4881
H -5.3915 3.9374 3.0254
H -3.9605 4.9952 3.0076
H -4.7086 4.5124 1.4711
O -6.6554 0.6490 -0.2237
C -6.9501 -0.4805 -1.0599
H -7.9800 -0.3414 -1.3752
H -6.2988 -0.4981 -1.9351
H -6.8608 -1.4128 -0.5006
39

trNHOts-li-N4

N 0.0868 1.4840 3.3886
O -1.5033 3.7159 4.7860
N -1.5791 1.2742 2.0342
O -3.6457 3.0447 5.4709
C -1.2437 1.1798 3.3773
C -2.5296 3.1510 5.0445
C -2.0873 0.9680 4.4527
H -1.6474 0.6750 5.3976
H -3.0872 0.6156 4.2399
N 0.5926 1.7305 2.1343
C -2.8718 1.0622 1.5021
C -0.4450 1.6102 1.3336
H -0.4236 1.7469 0.2648
C 0.9515 1.4682 4.5516
H 1.0730 0.4502 4.9250

H 0.5242 2.1003 5.3287
H 1.9154 1.8659 4.2468
C -4.4347 -0.2542 0.1881
C -5.3901 0.7510 0.3536
C -5.1097 1.9151 1.0909
C -3.8486 2.0718 1.6580
C -3.1762 -0.0991 0.7849
H -4.6278 -1.1653 -0.3594
H -5.8833 2.6642 1.1836
O -2.2540 -1.0909 0.5467
C -1.5673 -1.6422 1.6957
H -0.6267 -1.1234 1.8767
H -2.2010 -1.5976 2.5817
H -1.3608 -2.6800 1.4434
O -3.4264 3.1712 2.3442
C -4.3555 4.2622 2.4562
H -5.2363 3.9673 3.0275
H -3.8178 5.0418 2.9875
H -4.6428 4.6244 1.4679
O -6.6544 0.6981 -0.1664
C -6.9885 -0.4488 -0.9641
H -8.0140 -0.2862 -1.2818
H -6.3395 -0.5150 -1.8384
H -6.9290 -1.3644 -0.3744
39

trNHOadd-1i-N4

N 0.1310 1.6815 3.3630
O -1.7166 3.5410 5.0599
N -1.4648 1.3505 1.9744
O -3.8481 2.7296 5.2592
C -1.1794 1.4175 3.3021
C -2.6282 2.6704 4.9494
C -2.1476 1.2750 4.4018
H -1.6854 0.7350 5.2322
H -3.0003 0.6944 4.0509
N 0.7002 1.7736 2.1308
C -2.7660 1.1473 1.4352
C -0.3022 1.5719 1.2894
H -0.2327 1.5782 0.2141
C 0.9520 1.8408 4.5646
H 1.2693 0.8616 4.9178
H 0.3527 2.3643 5.3026
H 1.8129 2.4396 4.2842
C -4.3863 -0.2666 0.3256
C -5.3278 0.7595 0.4677
C -5.0032 1.9834 1.0811
C -3.7115 2.1861 1.5565

C -3.0961 -0.0632 0.8291
H -4.6181 -1.1954 -0.1744
H -5.7680 2.7441 1.1528
O -2.0977 -1.0007 0.6960
C -2.3577 -2.2459 1.3838
H -2.4683 -2.0639 2.4543
H -3.2496 -2.7362 0.9949
H -1.4877 -2.8698 1.1988
O -3.2411 3.3133 2.1467
C -4.1968 4.3477 2.4456
H -4.9754 3.9639 3.1031
H -3.6258 5.1131 2.9603
H -4.6187 4.7545 1.5254
O -6.6146 0.6785 0.0178
C -7.0113 -0.5357 -0.6407
H -8.0543 -0.3882 -0.9041
H -6.4243 -0.6957 -1.5460
H -6.9207 -1.3903 0.0310
35
trNHO_1e_N2_1e_N4
N 0.1883 1.6853 3.3249
N -1.4893 1.3281 1.9543
C -1.1646 1.3420 3.3240
C -1.9913 1.1075 4.3958
H -1.6084 1.1027 5.3996
H -3.0197 0.8305 4.2582
N 0.6956 1.7926 2.0444
C -0.3329 1.5888 1.2605
H -0.2734 1.6394 0.1890
C 1.1269 1.6825 4.4722
C 1.1857 0.2762 5.0726
C 2.5159 2.0706 3.9707
C 0.6806 2.7315 5.4940
H 2.8918 1.3620 3.2356
H 3.1908 2.0758 4.8281
H 2.5130 3.0656 3.5266
H 1.5610 -0.4277 4.3274
H 1.8624 0.2673 5.9290
H 0.6443 3.7151 5.0225
H 1.4017 2.7665 6.3124
H -0.2972 2.5205 5.9187
H 0.2079 -0.0667 5.4062
C -2.8102 1.0251 1.3445
C -3.8365 2.0526 1.8261
C -2.7008 1.1408 -0.1758
C -3.2107 -0.4095 1.6933
H -2.4177 2.1466 -0.4885

H -3.6822 0.9269 -0.5997
 H -1.9989 0.4184 -0.5939
 H -3.5183 3.0567 1.5401
 H -4.7998 1.8483 1.3559
 H -2.4739 -1.1086 1.2936
 H -4.1801 -0.6362 1.2464
 H -3.2845 -0.5681 2.7661
 H -3.9731 2.0316 2.9037
 38
 trNH0vdw_1e_N2_1e_N4
 N 0.1463 1.5740 3.4553
 O -1.7606 3.9872 3.6954
 N -1.5404 1.3177 2.0775
 O -3.1215 3.5022 5.5637
 C -1.1326 1.0246 3.3913
 C -2.4371 3.7270 4.6280
 C -1.8342 0.3678 4.3746
 H -1.4174 0.2334 5.3559
 H -2.8359 0.0170 4.2092
 N 0.5241 2.1534 2.2633
 C -0.5031 1.9812 1.4689
 H -0.5268 2.3344 0.4543
 C 1.1064 1.5313 4.5819
 C 1.4175 0.0727 4.9266
 C 2.3999 2.2185 4.1512
 C 0.5239 2.2930 5.7761
 H 2.8639 1.7057 3.3101
 H 3.0886 2.1937 4.9974
 H 2.2276 3.2571 3.8730
 H 1.8272 -0.4335 4.0506
 H 2.1598 0.0375 5.7259
 H 0.4123 3.3490 5.5244
 H 1.2056 2.2165 6.6253
 H -0.4428 1.9018 6.0874
 H 0.5376 -0.4739 5.2574
 C -2.8359 0.9698 1.4401
 C -3.9737 1.6700 2.1873
 C -2.8361 1.4672 -0.0052
 C -2.9974 -0.5517 1.4225
 H -2.7282 2.5510 -0.0656
 H -3.7975 1.2076 -0.4491
 H -2.0576 0.9900 -0.6017
 H -3.8676 2.7522 2.0959
 H -4.9294 1.3832 1.7451
 H -2.1689 -1.0045 0.8749
 H -3.9293 -0.8119 0.9179
 H -3.0205 -0.9798 2.4211

H -3.9995 1.4089 3.2427
 38
 trNHots_1e_N2_1e_N4
 N 0.1994 1.6199 3.3812
 O -1.9625 3.8869 4.0096
 N -1.4904 1.3757 2.0209
 O -3.3367 3.1429 5.7671
 C -1.1271 1.2395 3.3600
 C -2.5891 3.3050 4.8464
 C -1.9668 1.0269 4.4484
 H -1.5224 0.7956 5.4025
 H -2.9323 0.5810 4.2782
 N 0.6545 1.9779 2.1364
 C -0.3828 1.8217 1.3468
 H -0.3536 2.0238 0.2921
 C 1.1582 1.5677 4.5177
 C 1.2415 0.1255 5.0210
 C 2.5336 1.9978 4.0129
 C 0.7169 2.5403 5.6140
 H 2.8902 1.3486 3.2152
 H 3.2286 1.9334 4.8513
 H 2.5234 3.0244 3.6496
 H 1.5987 -0.5268 4.2221
 H 1.9455 0.0711 5.8532
 H 0.6340 3.5498 5.2098
 H 1.4682 2.5442 6.4056
 H -0.2348 2.2669 6.0637
 H 0.2803 -0.2491 5.3670
 C -2.7962 1.0199 1.3948
 C -3.9022 1.9153 1.9567
 C -2.7063 1.2601 -0.1121
 C -3.0671 -0.4661 1.6343
 H -2.5319 2.3102 -0.3502
 H -3.6626 0.9779 -0.5527
 H -1.9358 0.6464 -0.5798
 H -3.6509 2.9654 1.8022
 H -4.8327 1.7007 1.4284
 H -2.2755 -1.0667 1.1828
 H -4.0164 -0.7400 1.1712
 H -3.1234 -0.7119 2.6920
 H -4.0782 1.7513 3.0165
 38
 trNHOadd_1e_N2_1e_N4
 N 0.2046 1.6202 3.3535
 O -2.0766 3.7645 4.0677
 N -1.4673 1.3771 1.9964
 O -3.2331 2.9259 5.8586

C -1.1279 1.3942 3.3175
C -2.4959 2.8537 4.8364
C -2.0441 1.3892 4.4765
H -1.5671 0.9373 5.3422
H -2.9250 0.7864 4.2725
N 0.7227 1.7402 2.1065
C -0.3144 1.5945 1.2994
H -0.2413 1.6333 0.2289
C 1.1468 1.6457 4.5305
C 1.2203 0.2241 5.0859
C 2.5196 2.0740 4.0185
C 0.6676 2.6617 5.5664
H 2.9120 1.3834 3.2755
H 3.1958 2.0833 4.8736
H 2.4915 3.0757 3.5905
H 1.5684 -0.4668 4.3164
H 1.9276 0.2028 5.9162
H 0.4779 3.6283 5.1018
H 1.4578 2.7782 6.3093
H -0.2284 2.3486 6.0954
H 0.2585 -0.1261 5.4588
C -2.8131 1.0930 1.3745
C -3.8487 2.0866 1.8979
C -2.6895 1.2708 -0.1378
C -3.1770 -0.3588 1.6819
H -2.4208 2.2926 -0.4086
H -3.6658 1.0602 -0.5731
H -1.9814 0.5716 -0.5828
H -3.4933 3.1097 1.7837
H -4.7611 1.9622 1.3131
H -2.4268 -1.0370 1.2727
H -4.1375 -0.5870 1.2179
H -3.2715 -0.5502 2.7489
H -4.1062 1.9261 2.9409
41
trNHO_1e_N2_1j_N4
N 0.2423 1.6416 3.3930
N -1.4012 1.4276 1.9791
C -1.0865 1.2308 3.3331
C -1.9399 0.7028 4.2620
H -1.6616 0.5487 5.2893
H -2.9523 0.4837 3.9560
N 0.7265 2.0349 2.1570
C -0.2837 1.8994 1.3344
H -0.2607 2.1276 0.2810
C 1.1322 1.6565 4.5755
C 1.3153 0.2235 5.0790

C 2.4882 2.2233 4.1659
 C 0.5176 2.5603 5.6461
 H 2.9618 1.6138 3.3979
 H 3.1288 2.2311 5.0490
 H 2.3976 3.2428 3.7932
 H 1.7658 -0.3919 4.2981
 H 1.9758 0.2199 5.9480
 H 0.3902 3.5702 5.2522
 H 1.1808 2.6047 6.5116
 H -0.4525 2.1984 5.9814
 H 0.3695 -0.2292 5.3720
 C -2.6197 1.0831 1.3568
 C -3.8714 -0.2961 -0.1968
 C -4.9838 0.5203 0.0003
 C -4.9451 1.6101 0.8806
 C -3.7555 1.8982 1.5585
 C -2.6868 -0.0284 0.4997
 H -3.9059 -1.1475 -0.8652
 H -5.8275 2.2200 1.0139
 O -1.6000 -0.8266 0.2343
 C -0.8804 -1.3615 1.3720
 H -0.0157 -0.7430 1.6116
 H -1.5344 -1.4416 2.2404
 H -0.5416 -2.3502 1.0685
 O -3.5626 2.9549 2.3983
 C -4.6722 3.8487 2.5834
 H -5.5176 3.3313 3.0393
 H -4.3076 4.6167 3.2589
 H -4.9686 4.3015 1.6361
 H -5.9039 0.3060 -0.5308
 44
 trNHOvdw_1e_N2_1j_N4
 O -1.4145 4.2999 3.6021
 O -2.8576 3.7325 5.3827
 C -2.1409 3.9935 4.4809
 N 0.0988 1.6541 3.5417
 N -1.5240 1.5020 2.0908
 C -1.1990 1.1605 3.4145
 C -2.0233 0.4869 4.2707
 H -1.7359 0.2299 5.2747
 H -3.0222 0.2489 3.9365
 N 0.5773 2.1764 2.3519
 C -0.4192 2.0780 1.5086
 H -0.4033 2.4142 0.4842
 C 1.0221 1.4617 4.6821
 C 1.2629 -0.0358 4.8857
 C 2.3458 2.1517 4.3661

C 0.4155 2.1126 5.9278
 H 2.8365 1.7037 3.5037
 H 2.9976 2.0421 5.2345
 H 2.2024 3.2140 4.1697
 H 1.7117 -0.4654 3.9880
 H 1.9486 -0.1901 5.7209
 H 0.3397 3.1920 5.7854
 H 1.0647 1.9293 6.7859
 H -0.5715 1.7200 6.1641
 H 0.3393 -0.5719 5.0999
 C -2.6777 1.0833 1.3951
 C -3.7000 -0.2619 -0.3503
 C -4.9224 0.3534 -0.0855
 C -5.0478 1.3251 0.9155
 C -3.9224 1.6940 1.6618
 C -2.5792 0.0799 0.4142
 H -3.6027 -1.0249 -1.1126
 H -6.0121 1.7769 1.0987
 O -1.3837 -0.5261 0.1053
 C -0.6721 -1.1499 1.2026
 H 0.1062 -0.4885 1.5825
 H -1.3584 -1.4188 2.0060
 H -0.2132 -2.0464 0.7898
 O -3.9098 2.6511 2.6367
 C -5.1573 3.3197 2.8888
 H -5.9078 2.6175 3.2547
 H -4.9439 4.0526 3.6605
 H -5.5133 3.8279 1.9916
 H -5.7965 0.0794 -0.6643
 44
 trNHots_1e_N2_1j_N4
 O -1.9388 3.8635 4.7164
 O -3.9016 2.7189 5.2981
 C -2.8179 3.0733 4.9186
 N 0.2755 1.7971 3.3358
 N -1.3706 1.5129 1.9489
 C -1.0395 1.3912 3.2940
 C -1.9387 1.0513 4.2923
 H -1.5766 0.7292 5.2561
 H -2.8665 0.6071 3.9558
 N 0.7601 2.1048 2.0790
 C -0.2598 1.9392 1.2685
 H -0.2406 2.1125 0.2047
 C 1.2428 1.6302 4.4575
 C 1.3900 0.1340 4.7392
 C 2.5868 2.2119 4.0283
 C 0.7479 2.3952 5.6843

H 3.0028 1.6823 3.1737
H 3.2759 2.1123 4.8682
H 2.4988 3.2685 3.7756
H 1.7841 -0.3769 3.8586
H 2.0874 -0.0184 5.5650
H 0.6188 3.4505 5.4471
H 1.4935 2.3005 6.4756
H -0.1945 2.0134 6.0680
H 0.4379 -0.3222 5.0107
C -2.6056 1.1263 1.3742
C -3.9103 -0.4090 0.0322
C -5.0098 0.4384 0.1663
C -4.9316 1.6305 0.8979
C -3.7206 1.9806 1.5053
C -2.7022 -0.0755 0.6546
H -3.9726 -1.3322 -0.5304
H -5.8031 2.2650 0.9804
O -1.6238 -0.9030 0.4469
C -0.9141 -1.3712 1.6186
H -0.0572 -0.7331 1.8346
H -1.5787 -1.4170 2.4815
H -0.5613 -2.3705 1.3720
O -3.4863 3.1252 2.2063
C -4.5747 4.0592 2.3049
H -5.4152 3.6231 2.8456
H -4.1778 4.9019 2.8634
H -4.8871 4.3920 1.3140
H -5.9480 0.1734 -0.3067
44
trNHOadd_1e_N2_lj_N4
O -1.7308 3.6556 4.8617
O -3.8435 2.8003 5.0801
C -2.6167 2.7552 4.7900
N 0.2909 1.7113 3.3985
N -1.2936 1.3644 1.9857
C -1.0281 1.4443 3.3217
C -2.1031 1.3412 4.3292
H -1.7770 0.7952 5.2109
H -2.9253 0.7824 3.8824
N 0.8562 1.8116 2.1586
C -0.1324 1.5954 1.3109
H -0.0501 1.5923 0.2359
C 1.2293 1.9476 4.5507
C 2.4609 1.0803 4.2956
C 1.5712 3.4350 4.5339
C 0.5860 1.5536 5.8717
H 2.0470 3.7106 3.5925

H 2.2680 3.6472 5.3467
H 0.6646 4.0226 4.6736
H 2.9849 1.3847 3.3923
H 3.1391 1.1880 5.1429
H -0.2746 2.1786 6.0960
H 1.3312 1.7131 6.6519
H 0.3157 0.4972 5.8902
H 2.1836 0.0281 4.2081
C -2.5693 1.0849 1.4159
C -4.0832 -0.4714 0.3699
C -5.0529 0.5376 0.3741
C -4.8051 1.8154 0.8847
C -3.5384 2.0996 1.4095
C -2.8205 -0.1989 0.9100
H -4.3232 -1.4436 -0.0366
H -5.5833 2.5654 0.8651
O -1.7817 -1.0765 1.0119
C -2.0041 -2.4095 0.5133
H -2.8197 -2.8920 1.0527
H -2.2097 -2.3917 -0.5573
H -1.0751 -2.9393 0.7013
O -3.1254 3.2852 1.9249
C -4.1336 4.2862 2.1606
H -4.9143 3.8912 2.8088
H -3.6113 5.0926 2.6648
H -4.5457 4.6449 1.2164
H -6.0320 0.3196 -0.0359
45

trNHO_1e_N2_1i_N4
N 0.2867 1.5912 3.3748
N -1.4240 1.4967 2.0279
C -1.0900 1.3864 3.3873
C -1.9788 1.0975 4.3856
H -1.6837 0.9795 5.4130
H -3.0244 1.0101 4.1290
N 0.7795 1.7655 2.0919
C -0.2724 1.7160 1.3123
H -0.2552 1.8286 0.2402
C 1.2170 1.5335 4.5248
C 1.1977 0.1184 5.1069
C 2.6248 1.8631 4.0388
C 0.7919 2.5806 5.5565
H 2.9682 1.1516 3.2901
H 3.2956 1.8159 4.8981
H 2.6744 2.8661 3.6160
H 1.5492 -0.5965 4.3608
H 1.8598 0.0656 5.9734

H 0.7882 3.5718 5.0998
 H 1.5025 2.5835 6.3847
 H -0.1985 2.3858 5.9622
 H 0.1984 -0.1767 5.4236
 C -2.7010 1.2635 1.4783
 C -4.2134 -0.0825 0.1254
 C -5.2000 0.8907 0.2902
 C -4.9604 2.0558 1.0401
 C -3.7154 2.2359 1.6361
 C -2.9715 0.0979 0.7512
 H -4.3754 -0.9970 -0.4266
 H -5.7580 2.7791 1.1345
 O -2.0283 -0.8772 0.5276
 C -1.3203 -1.3852 1.6843
 H -0.3723 -0.8658 1.8200
 H -1.9305 -1.2927 2.5830
 H -1.1277 -2.4350 1.4721
 O -3.3452 3.3330 2.3553
 C -4.3275 4.3693 2.5123
 H -5.2008 3.9994 3.0515
 H -3.8363 5.1397 3.0991
 H -4.6218 4.7755 1.5434
 O -6.4562 0.8086 -0.2497
 C -6.7498 -0.3462 -1.0508
 H -7.7744 -0.2100 -1.3843
 H -6.0869 -0.3982 -1.9158
 H -6.6759 -1.2600 -0.4597
 48
 trNHOvdw_1e_N2_1i_N4
 O -1.3808 4.2773 4.3710
 O -3.3387 3.6389 5.5261
 C -2.3587 3.9222 4.9298
 N 0.2023 1.6475 3.4348
 N -1.5019 1.5749 2.0716
 C -1.1548 1.3344 3.4106
 C -2.0235 0.8858 4.3644
 H -1.7291 0.6909 5.3799
 H -3.0636 0.7724 4.0948
 N 0.6837 1.9550 2.1703
 C -0.3647 1.9242 1.3857
 H -0.3560 2.1509 0.3315
 C 1.1677 1.3161 4.5086
 C 1.1928 -0.2021 4.6999
 C 2.5512 1.8078 4.0914
 C 0.7645 2.0469 5.7915
 H 2.9084 1.2978 3.1990
 H 3.2429 1.6037 4.9104

H 2.5463 2.8809 3.8991
 H 1.5400 -0.6854 3.7845
 H 1.8766 -0.4664 5.5091
 H 0.7546 3.1235 5.6198
 H 1.4948 1.8254 6.5719
 H -0.2134 1.7459 6.1600
 H 0.2048 -0.5927 4.9443
 C -2.7547 1.2762 1.4967
 C -4.1628 -0.1376 0.0993
 C -5.2135 0.7638 0.2746
 C -5.0586 1.9248 1.0519
 C -3.8302 2.1805 1.6543
 C -2.9381 0.1152 0.7338
 H -4.2541 -1.0411 -0.4860
 H -5.9038 2.5910 1.1518
 O -1.9251 -0.7758 0.4689
 C -1.1540 -1.2718 1.5904
 H -0.2510 -0.6785 1.7299
 H -1.7504 -1.2705 2.5026
 H -0.8774 -2.2909 1.3265
 O -3.5412 3.3010 2.3814
 C -4.5553 4.3190 2.4181
 H -5.4319 3.9808 2.9725
 H -4.1028 5.1635 2.9305
 H -4.8350 4.6205 1.4077
 O -6.4583 0.6069 -0.2741
 C -6.6783 -0.5661 -1.0725
 H -7.7124 -0.5010 -1.3979
 H -6.0210 -0.5746 -1.9434
 H -6.5363 -1.4714 -0.4808
 48
 trNHOTs_1e_N2_1i_N4
 O -1.5879 4.0486 4.6097
 O -3.6349 3.2308 5.4117
 C -2.5466 3.4043 4.9325
 N 0.2613 1.6792 3.3661
 N -1.4409 1.5513 2.0225
 C -1.0935 1.4322 3.3639
 C -2.0017 1.2450 4.3930
 H -1.6599 0.9158 5.3616
 H -2.9904 0.9197 4.0959
 N 0.7499 1.8795 2.0886
 C -0.3026 1.8147 1.3061
 H -0.2888 1.9482 0.2364
 C 1.2286 1.4272 4.4717
 C 1.2040 -0.0678 4.7940
 C 2.6215 1.8334 3.9981

C 0.8604 2.2777 5.6870
H 2.9515 1.2361 3.1507
H 3.3139 1.6747 4.8261
H 2.6526 2.8862 3.7176
H 1.5101 -0.6456 3.9196
H 1.9000 -0.2812 5.6073
H 0.8488 3.3341 5.4214
H 1.6119 2.1172 6.4619
H -0.1085 2.0196 6.1063
H 0.2117 -0.3984 5.1015
C -2.7201 1.2840 1.4811
C -4.1996 -0.1291 0.1667
C -5.2039 0.8325 0.2997
C -4.9886 2.0213 1.0186
C -3.7456 2.2482 1.6030
C -2.9611 0.0963 0.7813
H -4.3405 -1.0578 -0.3670
H -5.7981 2.7343 1.0872
O -1.9868 -0.8539 0.5769
C -1.3258 -1.3779 1.7531
H -0.4196 -0.8151 1.9760
H -1.9982 -1.3664 2.6115
H -1.0581 -2.4036 1.5081
O -3.3913 3.3773 2.2780
C -4.3800 4.4164 2.3693
H -5.2537 4.0759 2.9259
H -3.8949 5.2252 2.9077
H -4.6688 4.7606 1.3750
O -6.4553 0.7118 -0.2397
C -6.7291 -0.4741 -1.0029
H -7.7567 -0.3673 -1.3376
H -6.0671 -0.5408 -1.8673
H -6.6369 -1.3660 -0.3820
48
trNHOadd_1e_N2_li_N4
O -1.5846 3.7060 4.9221
O -3.7779 3.0513 4.9681
C -2.5418 2.8916 4.7750
N 0.2933 1.6119 3.4171
N -1.3145 1.3964 2.0029
C -1.0426 1.4517 3.3393
C -2.1257 1.4368 4.3430
H -1.8401 0.8840 5.2343
H -2.9826 0.9305 3.8988
N 0.8651 1.6662 2.1769
C -0.1384 1.5335 1.3295
H -0.0548 1.5303 0.2549

C 1.2470 1.7753 4.5690
C 2.4066 0.8134 4.3166
C 1.7042 3.2314 4.5488
C 0.5746 1.4373 5.8911
H 2.2006 3.4667 3.6070
H 2.4147 3.3910 5.3617
H 0.8460 3.8884 4.6867
H 2.9528 1.0732 3.4125
H 3.0915 0.8702 5.1635
H -0.2336 2.1300 6.1119
H 1.3303 1.5393 6.6709
H 0.2214 0.4057 5.9128
H 2.0477 -0.2141 4.2323
C -2.6117 1.2474 1.4375
C -4.3325 -0.1712 0.4994
C -5.1770 0.9470 0.4647
C -4.7551 2.2163 0.8902
C -3.4651 2.3632 1.3934
C -3.0411 -0.0160 1.0193
H -4.6776 -1.1393 0.1764
H -5.4519 3.0406 0.8376
O -2.1258 -1.0175 1.1558
C -2.5373 -2.3413 0.7664
H -3.3808 -2.6749 1.3713
H -2.7851 -2.3720 -0.2949
H -1.6751 -2.9729 0.9590
O -2.9101 3.5210 1.8350
C -3.8000 4.6300 2.0610
H -4.5869 4.3440 2.7575
H -3.1791 5.4017 2.5051
H -4.2143 4.9892 1.1179
O -6.4602 0.9049 -0.0036
C -6.9525 -0.3530 -0.4931
H -7.9678 -0.1510 -0.8204
H -6.3581 -0.6990 -1.3394
H -6.9679 -1.1017 0.2999