Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information for:

The trianionic hydrazido radical $(N_2)^{3-}$: a promising platform for transforming N_2.

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Contents

DFT Calculations

Geometric structure optimizations were performed with TPSSh/def2-SVP level of theory by ORCA 5.0.3.[1,2] The wavefunctions were generated at the wB97M-V/def2-TZVP level of theory based on the optimized structures. The wave function analysis (FBO[3] and LOL[4]) was performed by the Multiwfn software.[5] We only took the anion component of **1** to simplify the calculation. The $S = {}^{1}/_{2}$ ground state was chosen for complex **1** and **1A**. To pair the α and β orbitals generated by the open shell calculations, biorthogonalization was performed based on the canonical orbitals by the Multiwfn software to obtain the SOMO of **1** and **1A**.

The Optimized Structures

1

CARTESIAN COORDINATES (ANGSTROEM)

Sc	2.829524	2.995092	3.230169
N	3.009669	3.054236	5.367463
N	2.305377	0.895559	2.909741
N	0.866886	2.536596	2.360273
C	1.065809	1.223601	2.523687
C	-0.033897	0.191592	2.353371
H	0.413851	-0.738737	1.978037
H	-0.741753	0.532674	1.584246
C	-0.798691	-0.084184	3.659821
H	-0.082071	-0.359392	4.450977
H	-1.274874	0.849813	3.995627
C	-1.862244	-1.180732	3.527632
H	-2.452979	-1.204855	4.459286
H	-2.569314	-0.906470	2.724135
C	-1.293259	-2.575689	3.260274
H	-0.751721	-2.622526	2.301775
H	-2.093602	-3.330989	3.221908
H	-0.588842	-2.872041	4.055302
C	-0.429445	3.106252	2.022588
H	-1.239642	2.509524	2.484754

C	-0.660196	3.119788	0.503633
H	0.104072	3.739892	0.010959
H	-1.651740	3.534957	0.260082
H	-0.596804	2.107150	0.075989
C	-0.516349	4.522209	2.598112
H	-0.348439	4.512917	3.683071
H	-1.501167	4.970511	2.392649
H	0.255056	5.161786	2.144503
C	2.721467	-0.474422	3.168376
H	1.878636	-1.059216	3.584421
C	3.183472	-1.169331	1.878201
H	2.385827	-1.173563	1.119269
H	3.478812	-2.212897	2.074480
H	4.047492	-0.638311	1.450061
C	3.835346	-0.465901	4.218262
H	4.707582	0.087399	3.839983
H	4.155364	-1.491173	4.461980
H	3.497254	0.029205	5.138630
C	5.079537	4.019657	3.179685
C	4.151324	5.032412	2.791160
C	3.571710	4.643107	1.546719
C	4.129518	3.382333	1.173733
C	5.074481	3.006051	2.175394
C	5.954174	4.070674	4.397338
H	5.393082	4.396884	5.286080
H	6.792710	4.776406	4.257827

H	6.386990	3.086090	4.623718
C	3.898807	6.305577	3.544688
H	2.974137	6.795917	3.208489
H	4.725741	7.024777	3.404955
H	3.801174	6.122727	4.625882
C	2.639181	5.462718	0.703216
H	1.934370	4.831294	0.143588
H	3.203956	6.056349	-0.037781
H	2.051630	6.171533	1.305096
C	3.803453	2.616951	-0.077424
H	4.050900	1.551017	0.028775
H	4.364759	3.003331	-0.946998
H	2.731781	2.683130	-0.320445
C	5.995142	1.821026	2.119750
H	6.290802	1.482828	3.124038
H	6.923073	2.074119	1.576513
H	5.537822	0.967354	1.599372
N	2.206319	3.952168	5.049331
Sc	2.387643	4.010713	7.186950
N	2.923019	6.105437	7.515576
N	4.354263	4.455057	8.056032
C	4.161825	5.769557	7.897844
C	5.266576	6.795831	8.070171
H	4.824019	7.725488	8.453301
H	5.976042	6.447091	8.834374
C	6.027660	7.077443	6.762743

H	5.309137	7.357274	5.974887
H	6.502131	6.144774	6.420940
C	7.092714	8.172269	6.897452
H	7.681637	8.199682	5.964746
H	7.801058	7.893767	7.698362
C	6.525946	9.566763	7.171838
H	5.986025	9.610183	8.131413
H	7.327337	10.320849	7.212188
H	5.820635	9.867486	6.379260
C	5.649443	3.877195	8.384487
H	6.460132	4.471632	7.920272
C	5.888740	3.856028	9.902027
H	5.124969	3.236704	10.396392
H	6.880040	3.435902	10.137983
H	5.831933	4.866924	10.334716
C	5.725479	2.463192	7.802607
H	5.551636	2.478082	6.718683
H	6.708842	2.008428	8.000771
H	4.952864	1.826022	8.257613
C	2.513070	7.478750	7.264820
H	3.358044	8.061486	6.850311
C	2.056797	8.169202	8.559372
H	2.855948	8.165846	9.316728
H	1.766004	9.215135	8.368975
H	1.191153	7.640048	8.986554
C	1.397436	7.481173	6.216765

H	0.522393	6.931655	6.594019
H	1.083226	8.509328	5.977693
H	1.731168	6.987808	5.293831
C	0.136424	2.989630	7.237616
C	1.062865	1.975845	7.627804
C	1.642584	2.365822	8.871912
C	1.086510	3.627815	9.243253
C	0.142585	4.004476	8.240775
C	-0.737525	2.938538	6.019435
H	-0.176099	2.611252	5.131284
H	-1.576812	2.233684	6.158859
H	-1.169267	3.923384	5.792078
C	1.313817	0.701349	6.876043
H	2.237467	0.209960	7.213502
H	0.485671	-0.016358	7.016256
H	1.412369	0.882635	5.794676
C	2.573215	1.546291	9.717538
H	3.281962	2.177353	10.272566
H	2.007277	0.958883	10.462605
H	3.156327	0.831900	9.117976
C	1.415408	4.393428	10.493587
H	1.148220	5.455245	10.395406
H	0.872130	3.993610	11.368478
H	2.491265	4.344663	10.722497
C	-0.775681	5.191550	8.293782
H	-1.070161	5.528379	7.288676

H	-1.704406	4.941533	8.837063
H	-0.316763	6.045377	8.812516

1A

CARTESIAN COORDINATES (ANGSTROEM)

Sc	0.230634	6.280049	4.414965
Sc	1.854889	2.711426	3.675190
N	1.008679	4.720981	3.391056
N	-1.814420	6.511586	3.682015
N	-1.449183	5.985971	5.851219
N	4.011962	2.287711	3.257607
N	3.311889	2.803199	5.330930
C	-2.337711	6.125245	4.855330
C	-1.905100	5.741612	7.215441
H	-2.916373	5.297810	7.188461
C	-1.998458	7.044411	8.025593
H	-2.590159	7.803125	7.494320
H	-0.997098	7.459469	8.201028
H	-2.467904	6.857763	9.005411
C	-1.005085	4.740707	7.935138
H	-1.397433	4.520889	8.940204
H	0.009308	5.146560	8.049946
H	-0.935958	3.797553	7.375869
C	-2.599723	6.599904	2.456797
H	-3.353716	5.789904	2.433458
C	-3.350235	7.934646	2.348901
H	-4.023697	8.084311	3.204266
H	-3.953596	7.971734	1.427543

H	-2.638487	8.773924	2.329429
C	-1.690141	6.376978	1.252734
H	-1.211006	5.392578	1.324071
H	-0.899991	7.141247	1.217319
H	-2.261478	6.425449	0.312667
C	0.580990	8.646131	5.016214
C	1.001837	8.509094	3.655802
C	2.159827	7.679351	3.631434
C	2.449904	7.291796	4.970972
C	1.489557	7.902786	5.831000
C	-0.585244	9.478931	5.468107
H	-0.434482	10.543635	5.218035
H	-0.732786	9.410127	6.554084
H	-1.523825	9.158823	4.985990
C	0.409568	9.254258	2.495063
H	-0.687868	9.284373	2.550148
H	0.686989	8.801920	1.531480
H	0.765505	10.300023	2.478835
C	3.068696	7.391818	2.473048
H	3.989154	7.998159	2.552790
H	2.602761	7.634712	1.508114
H	3.373339	6.334604	2.450518
C	3.658113	6.494484	5.373936
H	3.696863	6.341710	6.461402
H	4.586119	7.014940	5.078934
H	3.670525	5.502977	4.893572

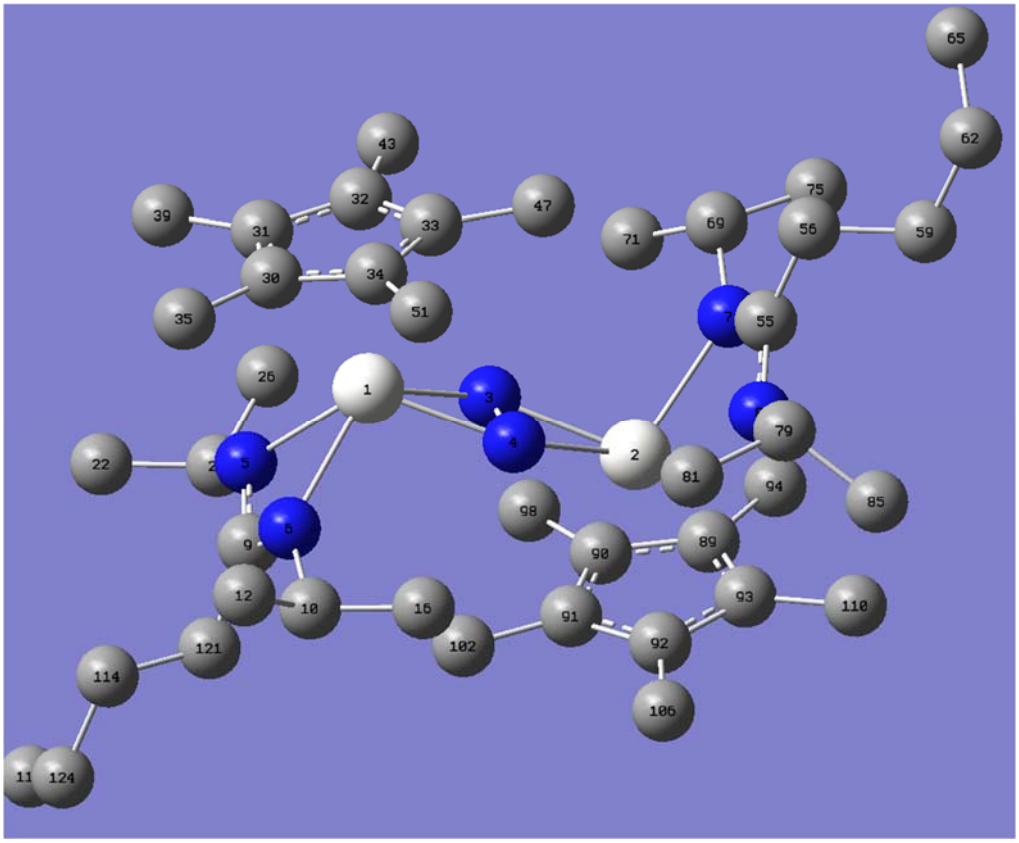
C	1.538645	7.865566	7.333437
H	2.514713	8.230557	7.694798
H	1.398815	6.855066	7.749049
H	0.766978	8.513225	7.770609
C	4.351734	2.651329	4.493195
C	5.787078	2.904879	4.920826
H	5.787346	3.456589	5.871279
H	6.262999	3.566587	4.179925
C	6.617422	1.619464	5.087655
H	6.035305	0.891990	5.676578
H	6.778733	1.152754	4.102671
C	7.971875	1.853048	5.767828
H	7.802419	2.273717	6.775639
H	8.457408	0.874408	5.923596
C	8.917987	2.765455	4.984838
H	9.100523	2.370060	3.971484
H	9.892317	2.854973	5.490181
H	8.508668	3.782713	4.876801
C	4.983366	2.159970	2.184050
H	5.962283	2.557989	2.508259
C	4.545566	2.988382	0.973397
H	3.564613	2.645694	0.608170
H	5.272920	2.898031	0.150624
H	4.452628	4.049296	1.248271
C	5.195566	0.689322	1.799407
H	5.491926	0.094306	2.676036

H	5.980869	0.595354	1.031572
H	4.267965	0.260195	1.397789
C	3.460249	3.228534	6.711803
H	4.232415	4.017840	6.794228
C	2.140744	3.843162	7.163711
H	2.214941	4.254444	8.181965
H	1.345342	3.087177	7.151792
H	1.846422	4.654046	6.478827
C	3.879393	2.081252	7.643921
H	3.137687	1.268632	7.611977
H	3.963276	2.432970	8.685314
H	4.851711	1.660815	7.348091
C	0.968734	0.677360	2.543755
C	-0.101968	1.615556	2.596889
C	-0.446425	1.822902	3.964457
C	0.414887	1.008722	4.759163
C	1.302689	0.312427	3.882214
C	1.555911	0.122976	1.276681
H	1.967709	0.907807	0.620961
H	0.787331	-0.413700	0.694382
H	2.362477	-0.591091	1.489869
C	-0.822835	2.204888	1.421762
H	-1.722338	1.615165	1.167588
H	-0.187586	2.233937	0.524326
H	-1.156978	3.231687	1.634063
C	-1.583259	2.681979	4.437100

H	-1.669973	3.589681	3.821113
H	-1.446677	3.007563	5.477168
H	-2.546328	2.142583	4.382110
C	0.323659	0.786114	6.240419
H	1.318126	0.730122	6.706499
H	-0.196325	-0.162993	6.462597
H	-0.240053	1.587359	6.740318
C	2.370218	-0.648415	4.322601
H	1.935621	-1.591600	4.698859
H	2.982034	-0.219599	5.132368
H	3.051381	-0.897768	3.497491
C	-4.672770	6.877647	5.694727
H	-4.446904	7.863687	5.253870
H	-4.394700	6.948640	6.756062
C	-6.757501	6.720676	4.183390
H	-6.596315	7.731430	3.773939
H	-6.296095	6.003208	3.486099
H	-7.841457	6.527216	4.182497
C	-3.814397	5.796228	5.013491
H	-3.902962	4.856202	5.581933
H	-4.222942	5.587958	4.016842
C	-6.179568	6.601574	5.595312
H	-6.706573	7.307825	6.259252
H	-6.387288	5.593520	5.997223
N	1.612673	4.248293	2.315799
C	1.456894	4.889110	1.029016

H	0.655559	4.401669	0.446024
H	1.201118	5.951952	1.140952
H	2.390300	4.794805	0.455472

Fuzzy atom bond order of complex **1**.



The total bond order >= 0.050000

#	1:	1(Sc)	2(Sc)	Alpha:	0.142861	Beta: 0.146961 Total: 0.289822
#	2:	1(Sc)	3(N)	Alpha:	0.561225	Beta: 0.521169 Total: 1.082394
#	3:	1(Sc)	4(N)	Alpha:	0.588007	Beta: 0.537251 Total: 1.125259
#	4:	1(Sc)	5(N)	Alpha:	0.444609	Beta: 0.448145 Total: 0.892754
#	5:	1(Sc)	6(N)	Alpha:	0.429911	Beta: 0.433866 Total: 0.863778
#	6:	1(Sc)	9(C)	Alpha:	0.120184	Beta: 0.120569 Total: 0.240753
#	7:	1(Sc)	10(C)	Alpha:	0.025005	Beta: 0.025244 Total: 0.050249
#	8:	1(Sc)	20(C)	Alpha:	0.025817	Beta: 0.025911 Total: 0.051728
#	9:	1(Sc)	30(C)	Alpha:	0.260122	Beta: 0.260760 Total: 0.520882
#	10:	1(Sc)	31(C)	Alpha:	0.259774	Beta: 0.261172 Total: 0.520945
#	11:	1(Sc)	32(C)	Alpha:	0.261240	Beta: 0.263759 Total: 0.524999
#	12:	1(Sc)	33(C)	Alpha:	0.257668	Beta: 0.257648 Total: 0.515317
#	13:	1(Sc)	34(C)	Alpha:	0.263247	Beta: 0.266143 Total: 0.529390
#	14:	1(Sc)	35(C)	Alpha:	0.025488	Beta: 0.025534 Total: 0.051022
#	15:	1(Sc)	51(C)	Alpha:	0.028503	Beta: 0.028667 Total: 0.057169
#	16:	2(Sc)	3(N)	Alpha:	0.564071	Beta: 0.522607 Total: 1.086678
#	17:	2(Sc)	4(N)	Alpha:	0.591974	Beta: 0.535237 Total: 1.127211
#	18:	2(Sc)	7(N)	Alpha:	0.447292	Beta: 0.450413 Total: 0.897705
#	19:	2(Sc)	8(N)	Alpha:	0.409842	Beta: 0.413862 Total: 0.823704

20: 2(Sc) 55(C) Alpha: 0.116721 Beta: 0.117121 Total: 0.233843
21: 2(Sc) 69(C) Alpha: 0.025967 Beta: 0.026045 Total: 0.052011
22: 2(Sc) 89(C) Alpha: 0.258101 Beta: 0.259266 Total: 0.517368
23: 2(Sc) 90(C) Alpha: 0.258639 Beta: 0.261304 Total: 0.519944
24: 2(Sc) 91(C) Alpha: 0.256187 Beta: 0.256094 Total: 0.512282
25: 2(Sc) 92(C) Alpha: 0.262870 Beta: 0.265420 Total: 0.528290
26: 2(Sc) 93(C) Alpha: 0.258290 Beta: 0.258859 Total: 0.517149
27: 2(Sc) 106(C) Alpha: 0.027478 Beta: 0.027646 Total: 0.055124
28: 2(Sc) 110(C) Alpha: 0.025471 Beta: 0.025527 Total: 0.050998
29: 3(N) 4(N) Alpha: 0.495466 Beta: 0.674841 Total: 1.170307
30: 5(N) 6(N) Alpha: 0.083732 Beta: 0.082798 Total: 0.166531
31: 5(N) 9(C) Alpha: 0.699141 Beta: 0.698397 Total: 1.397537
32: 5(N) 20(C) Alpha: 0.547929 Beta: 0.547776 Total: 1.095705
33: 5(N) 22(C) Alpha: 0.048707 Beta: 0.048588 Total: 0.097294
34: 5(N) 26(C) Alpha: 0.045555 Beta: 0.045760 Total: 0.091314
35: 5(N) 121(C) Alpha: 0.035883 Beta: 0.035816 Total: 0.071700
36: 6(N) 9(C) Alpha: 0.713788 Beta: 0.713908 Total: 1.427696
37: 6(N) 10(C) Alpha: 0.546871 Beta: 0.546414 Total: 1.093285
38: 6(N) 12(C) Alpha: 0.054047 Beta: 0.053907 Total: 0.107954
39: 6(N) 16(C) Alpha: 0.044442 Beta: 0.044717 Total: 0.089159
40: 6(N) 121(C) Alpha: 0.036209 Beta: 0.036216 Total: 0.072425
41: 7(N) 8(N) Alpha: 0.084180 Beta: 0.083378 Total: 0.167558
42: 7(N) 55(C) Alpha: 0.698018 Beta: 0.697094 Total: 1.395112
43: 7(N) 56(C) Alpha: 0.035813 Beta: 0.035729 Total: 0.071542
44: 7(N) 69(C) Alpha: 0.547940 Beta: 0.547877 Total: 1.095817
45: 7(N) 71(C) Alpha: 0.045300 Beta: 0.045557 Total: 0.090857
46: 7(N) 75(C) Alpha: 0.049411 Beta: 0.049328 Total: 0.098739
47: 8(N) 55(C) Alpha: 0.719927 Beta: 0.720261 Total: 1.440187
48: 8(N) 56(C) Alpha: 0.036541 Beta: 0.036569 Total: 0.073111
49: 8(N) 79(C) Alpha: 0.548291 Beta: 0.547768 Total: 1.096059
50: 8(N) 81(C) Alpha: 0.044709 Beta: 0.044942 Total: 0.089651
51: 8(N) 85(C) Alpha: 0.053816 Beta: 0.053658 Total: 0.107474
52: 9(C) 10(C) Alpha: 0.036443 Beta: 0.036439 Total: 0.072882
53: 9(C) 20(C) Alpha: 0.035272 Beta: 0.035241 Total: 0.070514
54: 9(C) 114(C) Alpha: 0.042814 Beta: 0.042800 Total: 0.085614
55: 9(C) 121(C) Alpha: 0.517188 Beta: 0.517210 Total: 1.034398
56: 10(C) 11(H) Alpha: 0.397896 Beta: 0.397908 Total: 0.795804
57: 10(C) 12(C) Alpha: 0.544286 Beta: 0.544206 Total: 1.088492
58: 10(C) 16(C) Alpha: 0.538506 Beta: 0.538293 Total: 1.076799
59: 12(C) 13(H) Alpha: 0.442845 Beta: 0.442838 Total: 0.885684
60: 12(C) 14(H) Alpha: 0.437477 Beta: 0.437474 Total: 0.874951
61: 12(C) 15(H) Alpha: 0.454064 Beta: 0.454051 Total: 0.908115
62: 12(C) 16(C) Alpha: 0.046200 Beta: 0.046095 Total: 0.092295

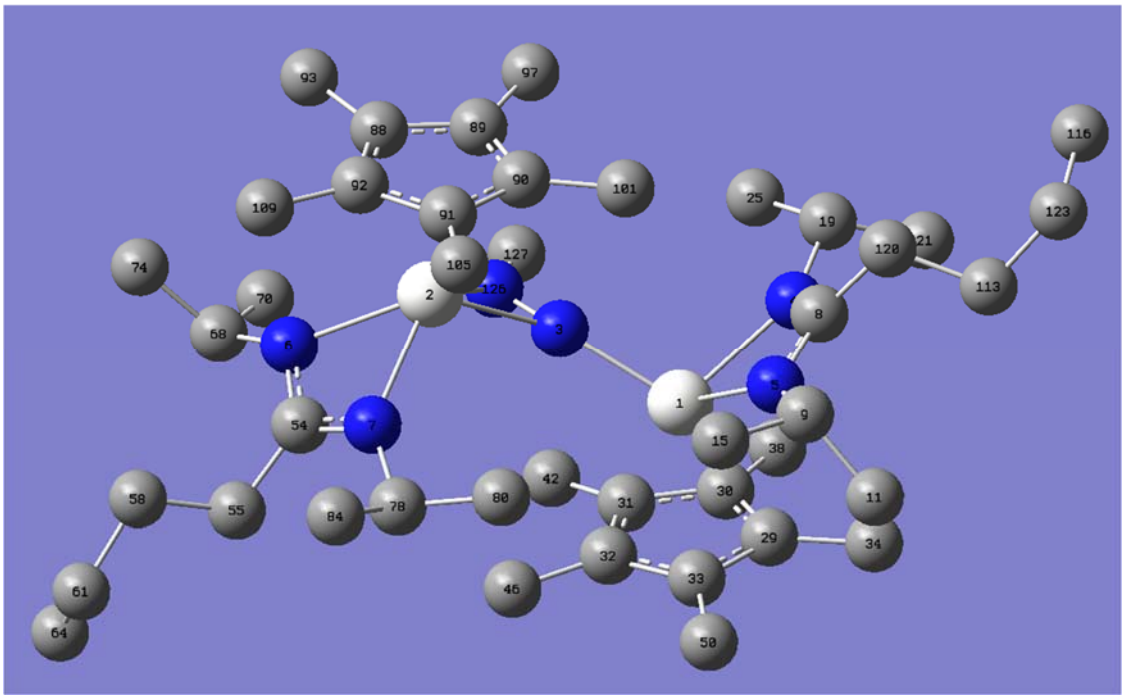
63: 16(C) 17(H) Alpha: 0.453168 Beta: 0.453033 Total: 0.906201
64: 16(C) 18(H) Alpha: 0.432078 Beta: 0.432052 Total: 0.864130
65: 16(C) 19(H) Alpha: 0.421199 Beta: 0.421641 Total: 0.842839
66: 20(C) 21(H) Alpha: 0.401698 Beta: 0.401702 Total: 0.803400
67: 20(C) 22(C) Alpha: 0.543554 Beta: 0.543526 Total: 1.087080
68: 20(C) 26(C) Alpha: 0.538967 Beta: 0.539055 Total: 1.078022
69: 22(C) 23(H) Alpha: 0.437541 Beta: 0.437542 Total: 0.875083
70: 22(C) 24(H) Alpha: 0.452648 Beta: 0.452645 Total: 0.905293
71: 22(C) 25(H) Alpha: 0.442775 Beta: 0.442774 Total: 0.885549
72: 22(C) 26(C) Alpha: 0.046678 Beta: 0.046630 Total: 0.093308
73: 26(C) 27(H) Alpha: 0.418056 Beta: 0.418155 Total: 0.836211
74: 26(C) 28(H) Alpha: 0.433648 Beta: 0.433557 Total: 0.867205
75: 26(C) 29(H) Alpha: 0.452961 Beta: 0.452924 Total: 0.905885
76: 30(C) 31(C) Alpha: 0.562342 Beta: 0.563822 Total: 1.126165
77: 30(C) 32(C) Alpha: 0.046870 Beta: 0.046572 Total: 0.093441
78: 30(C) 33(C) Alpha: 0.047440 Beta: 0.047500 Total: 0.094941
79: 30(C) 34(C) Alpha: 0.564670 Beta: 0.562549 Total: 1.127219
80: 30(C) 35(C) Alpha: 0.554832 Beta: 0.554824 Total: 1.109656
81: 30(C) 39(C) Alpha: 0.029395 Beta: 0.029489 Total: 0.058884
82: 30(C) 51(C) Alpha: 0.029306 Beta: 0.029206 Total: 0.058512
83: 31(C) 32(C) Alpha: 0.565437 Beta: 0.563472 Total: 1.128910
84: 31(C) 33(C) Alpha: 0.046976 Beta: 0.046985 Total: 0.093960
85: 31(C) 34(C) Alpha: 0.047036 Beta: 0.046356 Total: 0.093392
86: 31(C) 35(C) Alpha: 0.029279 Beta: 0.029385 Total: 0.058664
87: 31(C) 39(C) Alpha: 0.556325 Beta: 0.556060 Total: 1.112385
88: 31(C) 42(H) Alpha: 0.025022 Beta: 0.025028 Total: 0.050050
89: 31(C) 43(C) Alpha: 0.029081 Beta: 0.029039 Total: 0.058120
90: 32(C) 33(C) Alpha: 0.561877 Beta: 0.561816 Total: 1.123693
91: 32(C) 34(C) Alpha: 0.046098 Beta: 0.045724 Total: 0.091822
92: 32(C) 39(C) Alpha: 0.028996 Beta: 0.028852 Total: 0.057848
93: 32(C) 43(C) Alpha: 0.555128 Beta: 0.555011 Total: 1.110140
94: 32(C) 44(H) Alpha: 0.025131 Beta: 0.025111 Total: 0.050242
95: 32(C) 47(C) Alpha: 0.028334 Beta: 0.028383 Total: 0.056717
96: 33(C) 34(C) Alpha: 0.563870 Beta: 0.564068 Total: 1.127938
97: 33(C) 43(C) Alpha: 0.028522 Beta: 0.028547 Total: 0.057069
98: 33(C) 47(C) Alpha: 0.552830 Beta: 0.552871 Total: 1.105701
99: 33(C) 51(C) Alpha: 0.029104 Beta: 0.029144 Total: 0.058248
100: 34(C) 35(C) Alpha: 0.028661 Beta: 0.028525 Total: 0.057186
101: 34(C) 47(C) Alpha: 0.027999 Beta: 0.028092 Total: 0.056091
102: 34(C) 51(C) Alpha: 0.553309 Beta: 0.553128 Total: 1.106437
103: 35(C) 36(H) Alpha: 0.446119 Beta: 0.446109 Total: 0.892227
104: 35(C) 37(H) Alpha: 0.437433 Beta: 0.437438 Total: 0.874871
105: 35(C) 38(H) Alpha: 0.433886 Beta: 0.433847 Total: 0.867734

106: 39(C) 40(H) Alpha: 0.431426 Beta: 0.431334 Total: 0.862760
107: 39(C) 41(H) Alpha: 0.438091 Beta: 0.438101 Total: 0.876192
108: 39(C) 42(H) Alpha: 0.446630 Beta: 0.446501 Total: 0.893130
109: 43(C) 44(H) Alpha: 0.447115 Beta: 0.447038 Total: 0.894154
110: 43(C) 45(H) Alpha: 0.441939 Beta: 0.441885 Total: 0.883824
111: 43(C) 46(H) Alpha: 0.428168 Beta: 0.428494 Total: 0.856662
112: 47(C) 48(H) Alpha: 0.432376 Beta: 0.431830 Total: 0.864206
113: 47(C) 49(H) Alpha: 0.444066 Beta: 0.444110 Total: 0.888176
114: 47(C) 50(H) Alpha: 0.411102 Beta: 0.411493 Total: 0.822595
115: 51(C) 52(H) Alpha: 0.446930 Beta: 0.446946 Total: 0.893876
116: 51(C) 53(H) Alpha: 0.438183 Beta: 0.438274 Total: 0.876458
117: 51(C) 54(H) Alpha: 0.438867 Beta: 0.438858 Total: 0.877725
118: 55(C) 56(C) Alpha: 0.517058 Beta: 0.517076 Total: 1.034133
119: 55(C) 59(C) Alpha: 0.042315 Beta: 0.042302 Total: 0.084616
120: 55(C) 69(C) Alpha: 0.034862 Beta: 0.034821 Total: 0.069683
121: 55(C) 79(C) Alpha: 0.036488 Beta: 0.036495 Total: 0.072983
122: 56(C) 57(H) Alpha: 0.411097 Beta: 0.411114 Total: 0.822211
123: 56(C) 58(H) Alpha: 0.407012 Beta: 0.407011 Total: 0.814022
124: 56(C) 59(C) Alpha: 0.545994 Beta: 0.546004 Total: 1.091998
125: 56(C) 62(C) Alpha: 0.038833 Beta: 0.038833 Total: 0.077666
126: 59(C) 60(H) Alpha: 0.418842 Beta: 0.418834 Total: 0.837676
127: 59(C) 61(H) Alpha: 0.420470 Beta: 0.420473 Total: 0.840942
128: 59(C) 62(C) Alpha: 0.560823 Beta: 0.560826 Total: 1.121649
129: 59(C) 65(C) Alpha: 0.041412 Beta: 0.041412 Total: 0.082824
130: 62(C) 63(H) Alpha: 0.430916 Beta: 0.430916 Total: 0.861832
131: 62(C) 64(H) Alpha: 0.435338 Beta: 0.435339 Total: 0.870677
132: 62(C) 65(C) Alpha: 0.583940 Beta: 0.583939 Total: 1.167879
133: 62(C) 67(H) Alpha: 0.025071 Beta: 0.025071 Total: 0.050142
134: 65(C) 66(H) Alpha: 0.450143 Beta: 0.450143 Total: 0.900285
135: 65(C) 67(H) Alpha: 0.457400 Beta: 0.457400 Total: 0.914800
136: 65(C) 68(H) Alpha: 0.447033 Beta: 0.447033 Total: 0.894066
137: 69(C) 70(H) Alpha: 0.401295 Beta: 0.401299 Total: 0.802594
138: 69(C) 71(C) Alpha: 0.539161 Beta: 0.539203 Total: 1.078364
139: 69(C) 75(C) Alpha: 0.543129 Beta: 0.543108 Total: 1.086237
140: 71(C) 72(H) Alpha: 0.434039 Beta: 0.433934 Total: 0.867974
141: 71(C) 73(H) Alpha: 0.452636 Beta: 0.452546 Total: 0.905183
142: 71(C) 74(H) Alpha: 0.418064 Beta: 0.418363 Total: 0.836427
143: 71(C) 75(C) Alpha: 0.046745 Beta: 0.046678 Total: 0.093423
144: 75(C) 76(H) Alpha: 0.438459 Beta: 0.438459 Total: 0.876918
145: 75(C) 77(H) Alpha: 0.453153 Beta: 0.453160 Total: 0.906313
146: 75(C) 78(H) Alpha: 0.442354 Beta: 0.442355 Total: 0.884709
147: 79(C) 80(H) Alpha: 0.397592 Beta: 0.397601 Total: 0.795193
148: 79(C) 81(C) Alpha: 0.538784 Beta: 0.538634 Total: 1.077418

149: 79(C) 85(C) Alpha: 0.544283 Beta: 0.544193 Total: 1.088475
150: 81(C) 82(H) Alpha: 0.453657 Beta: 0.453556 Total: 0.907213
151: 81(C) 83(H) Alpha: 0.432929 Beta: 0.432854 Total: 0.865783
152: 81(C) 84(H) Alpha: 0.420783 Beta: 0.421223 Total: 0.842007
153: 81(C) 85(C) Alpha: 0.046292 Beta: 0.046189 Total: 0.092481
154: 85(C) 86(H) Alpha: 0.437235 Beta: 0.437232 Total: 0.874467
155: 85(C) 87(H) Alpha: 0.454267 Beta: 0.454244 Total: 0.908511
156: 85(C) 88(H) Alpha: 0.443456 Beta: 0.443452 Total: 0.886908
157: 89(C) 90(C) Alpha: 0.566717 Beta: 0.564570 Total: 1.131287
158: 89(C) 91(C) Alpha: 0.047127 Beta: 0.047163 Total: 0.094290
159: 89(C) 92(C) Alpha: 0.046939 Beta: 0.046404 Total: 0.093343
160: 89(C) 93(C) Alpha: 0.563033 Beta: 0.564701 Total: 1.127734
161: 89(C) 94(C) Alpha: 0.556575 Beta: 0.556338 Total: 1.112913
162: 89(C) 96(H) Alpha: 0.025043 Beta: 0.025049 Total: 0.050093
163: 89(C) 98(C) Alpha: 0.029204 Beta: 0.029125 Total: 0.058329
164: 89(C) 110(C) Alpha: 0.029339 Beta: 0.029454 Total: 0.058793
165: 90(C) 91(C) Alpha: 0.562196 Beta: 0.562253 Total: 1.124449
166: 90(C) 92(C) Alpha: 0.046105 Beta: 0.045770 Total: 0.091875
167: 90(C) 93(C) Alpha: 0.046982 Beta: 0.046624 Total: 0.093606
168: 90(C) 94(C) Alpha: 0.029085 Beta: 0.028923 Total: 0.058008
169: 90(C) 98(C) Alpha: 0.555557 Beta: 0.555389 Total: 1.110946
170: 90(C) 99(H) Alpha: 0.025131 Beta: 0.025113 Total: 0.050244
171: 90(C) 102(C) Alpha: 0.028226 Beta: 0.028317 Total: 0.056543
172: 91(C) 92(C) Alpha: 0.564281 Beta: 0.564478 Total: 1.128760
173: 91(C) 93(C) Alpha: 0.047699 Beta: 0.047770 Total: 0.095469
174: 91(C) 98(C) Alpha: 0.028448 Beta: 0.028485 Total: 0.056932
175: 91(C) 102(C) Alpha: 0.553168 Beta: 0.553131 Total: 1.106299
176: 91(C) 106(C) Alpha: 0.029108 Beta: 0.029144 Total: 0.058252
177: 92(C) 93(C) Alpha: 0.564834 Beta: 0.562790 Total: 1.127624
178: 92(C) 102(C) Alpha: 0.028165 Beta: 0.028216 Total: 0.056381
179: 92(C) 106(C) Alpha: 0.553867 Beta: 0.553759 Total: 1.107625
180: 92(C) 110(C) Alpha: 0.028714 Beta: 0.028583 Total: 0.057298
181: 93(C) 94(C) Alpha: 0.029431 Beta: 0.029540 Total: 0.058970
182: 93(C) 106(C) Alpha: 0.029354 Beta: 0.029275 Total: 0.058629
183: 93(C) 110(C) Alpha: 0.555404 Beta: 0.555358 Total: 1.110762
184: 94(C) 95(H) Alpha: 0.438900 Beta: 0.438909 Total: 0.877809
185: 94(C) 96(H) Alpha: 0.446876 Beta: 0.446758 Total: 0.893634
186: 94(C) 97(H) Alpha: 0.431443 Beta: 0.431364 Total: 0.862807
187: 98(C) 99(H) Alpha: 0.447365 Beta: 0.447325 Total: 0.894691
188: 98(C) 100(H) Alpha: 0.442096 Beta: 0.442033 Total: 0.884129
189: 98(C) 101(H) Alpha: 0.427802 Beta: 0.428184 Total: 0.855986
190: 102(C) 103(H) Alpha: 0.409925 Beta: 0.410545 Total: 0.820470
191: 102(C) 104(H) Alpha: 0.433165 Beta: 0.432668 Total: 0.865833

192: 102(C) 105(H) Alpha: 0.443693 Beta: 0.443757 Total: 0.887450
193: 106(C) 107(H) Alpha: 0.439669 Beta: 0.439665 Total: 0.879334
194: 106(C) 108(H) Alpha: 0.446810 Beta: 0.446831 Total: 0.893641
195: 106(C) 109(H) Alpha: 0.437623 Beta: 0.437704 Total: 0.875327
196: 110(C) 111(H) Alpha: 0.446134 Beta: 0.446101 Total: 0.892235
197: 110(C) 112(H) Alpha: 0.437440 Beta: 0.437446 Total: 0.874886
198: 110(C) 113(H) Alpha: 0.433439 Beta: 0.433378 Total: 0.866817
199: 114(C) 115(H) Alpha: 0.419598 Beta: 0.419601 Total: 0.839199
200: 114(C) 116(H) Alpha: 0.419338 Beta: 0.419330 Total: 0.838668
201: 114(C) 117(C) Alpha: 0.041528 Beta: 0.041528 Total: 0.083056
202: 114(C) 121(C) Alpha: 0.546524 Beta: 0.546536 Total: 1.093060
203: 114(C) 124(C) Alpha: 0.560723 Beta: 0.560726 Total: 1.121449
204: 117(C) 118(H) Alpha: 0.449672 Beta: 0.449672 Total: 0.899344
205: 117(C) 119(H) Alpha: 0.446348 Beta: 0.446348 Total: 0.892697
206: 117(C) 120(H) Alpha: 0.457542 Beta: 0.457542 Total: 0.915083
207: 117(C) 124(C) Alpha: 0.584099 Beta: 0.584099 Total: 1.168198
208: 120(H) 124(C) Alpha: 0.025049 Beta: 0.025049 Total: 0.050098
209: 121(C) 122(H) Alpha: 0.412633 Beta: 0.412655 Total: 0.825288
210: 121(C) 123(H) Alpha: 0.406484 Beta: 0.406482 Total: 0.812966
211: 121(C) 124(C) Alpha: 0.039020 Beta: 0.039020 Total: 0.078040
212: 124(C) 125(H) Alpha: 0.435142 Beta: 0.435143 Total: 0.870285
213: 124(C) 126(H) Alpha: 0.430943 Beta: 0.430943 Total: 0.861885

Fuzzy atom bond order of complex **1A**.



The total bond order >= 0.050000

1: 1(Sc) 2(Sc) Alpha: 0.077592 Beta: 0.071423 Total: 0.149015
2: 1(Sc) 3(N) Alpha: 0.768016 Beta: 0.559571 Total: 1.327587
3: 1(Sc) 4(N) Alpha: 0.479850 Beta: 0.482278 Total: 0.962128
4: 1(Sc) 5(N) Alpha: 0.454048 Beta: 0.453792 Total: 0.907839
5: 1(Sc) 8(C) Alpha: 0.116875 Beta: 0.121220 Total: 0.238095
6: 1(Sc) 9(C) Alpha: 0.025911 Beta: 0.025963 Total: 0.051874
7: 1(Sc) 19(C) Alpha: 0.027158 Beta: 0.027410 Total: 0.054568
8: 1(Sc) 29(C) Alpha: 0.279645 Beta: 0.280817 Total: 0.560462
9: 1(Sc) 30(C) Alpha: 0.284147 Beta: 0.284593 Total: 0.568740
10: 1(Sc) 31(C) Alpha: 0.268100 Beta: 0.268633 Total: 0.536732
11: 1(Sc) 32(C) Alpha: 0.270336 Beta: 0.270451 Total: 0.540787
12: 1(Sc) 33(C) Alpha: 0.276451 Beta: 0.277696 Total: 0.554147
13: 1(Sc) 34(C) Alpha: 0.027691 Beta: 0.027943 Total: 0.055634
14: 1(Sc) 50(C) Alpha: 0.025254 Beta: 0.025335 Total: 0.050589
15: 1(Sc) 126(N) Alpha: 0.080822 Beta: 0.070704 Total: 0.151526
16: 2(Sc) 3(N) Alpha: 0.441860 Beta: 0.451583 Total: 0.893443
17: 2(Sc) 6(N) Alpha: 0.440472 Beta: 0.443115 Total: 0.883587
18: 2(Sc) 7(N) Alpha: 0.461484 Beta: 0.462731 Total: 0.924215
19: 2(Sc) 54(C) Alpha: 0.115082 Beta: 0.115232 Total: 0.230314
20: 2(Sc) 68(C) Alpha: 0.025073 Beta: 0.025227 Total: 0.050300
21: 2(Sc) 78(C) Alpha: 0.026042 Beta: 0.026152 Total: 0.052193
22: 2(Sc) 88(C) Alpha: 0.278646 Beta: 0.279570 Total: 0.558217

23: 2(Sc) 89(C) Alpha: 0.272987 Beta: 0.273451 Total: 0.546438
24: 2(Sc) 90(C) Alpha: 0.271726 Beta: 0.272512 Total: 0.544238
25: 2(Sc) 91(C) Alpha: 0.277929 Beta: 0.278636 Total: 0.556564
26: 2(Sc) 92(C) Alpha: 0.278452 Beta: 0.278674 Total: 0.557126
27: 2(Sc) 93(C) Alpha: 0.031097 Beta: 0.031140 Total: 0.062238
28: 2(Sc) 109(C) Alpha: 0.028580 Beta: 0.028565 Total: 0.057145
29: 2(Sc) 126(N) Alpha: 0.599336 Beta: 0.538224 Total: 1.137560
30: 2(Sc) 127(C) Alpha: 0.040765 Beta: 0.038614 Total: 0.079379
31: 3(N) 126(N) Alpha: 0.593757 Beta: 0.805651 Total: 1.399408
32: 3(N) 127(C) Alpha: 0.042710 Beta: 0.051747 Total: 0.094456
33: 4(N) 5(N) Alpha: 0.080985 Beta: 0.080391 Total: 0.161376
34: 4(N) 8(C) Alpha: 0.702329 Beta: 0.698561 Total: 1.400891
35: 4(N) 19(C) Alpha: 0.538747 Beta: 0.538857 Total: 1.077604
36: 4(N) 21(C) Alpha: 0.048766 Beta: 0.048749 Total: 0.097515
37: 4(N) 25(C) Alpha: 0.046007 Beta: 0.046237 Total: 0.092244
38: 4(N) 120(C) Alpha: 0.035366 Beta: 0.035173 Total: 0.070539
39: 5(N) 8(C) Alpha: 0.705410 Beta: 0.705518 Total: 1.410929
40: 5(N) 9(C) Alpha: 0.540262 Beta: 0.540264 Total: 1.080526
41: 5(N) 11(C) Alpha: 0.049723 Beta: 0.049741 Total: 0.099464
42: 5(N) 15(C) Alpha: 0.047332 Beta: 0.047330 Total: 0.094662
43: 5(N) 120(C) Alpha: 0.035589 Beta: 0.035615 Total: 0.071204
44: 6(N) 7(N) Alpha: 0.083000 Beta: 0.082695 Total: 0.165695
45: 6(N) 54(C) Alpha: 0.720552 Beta: 0.719929 Total: 1.440481
46: 6(N) 55(C) Alpha: 0.036195 Beta: 0.036153 Total: 0.072348
47: 6(N) 68(C) Alpha: 0.541672 Beta: 0.541376 Total: 1.083049
48: 6(N) 70(C) Alpha: 0.047289 Beta: 0.047403 Total: 0.094692
49: 6(N) 74(C) Alpha: 0.051988 Beta: 0.051947 Total: 0.103935
50: 7(N) 54(C) Alpha: 0.693603 Beta: 0.693930 Total: 1.387533
51: 7(N) 55(C) Alpha: 0.034843 Beta: 0.034849 Total: 0.069692
52: 7(N) 78(C) Alpha: 0.544951 Beta: 0.544777 Total: 1.089728
53: 7(N) 80(C) Alpha: 0.047944 Beta: 0.047971 Total: 0.095915
54: 7(N) 84(C) Alpha: 0.047328 Beta: 0.047289 Total: 0.094617
55: 8(C) 9(C) Alpha: 0.036291 Beta: 0.036288 Total: 0.072579
56: 8(C) 19(C) Alpha: 0.034599 Beta: 0.034426 Total: 0.069025
57: 8(C) 113(C) Alpha: 0.041205 Beta: 0.041340 Total: 0.082544
58: 8(C) 120(C) Alpha: 0.520979 Beta: 0.520814 Total: 1.041792
59: 9(C) 10(H) Alpha: 0.393895 Beta: 0.393908 Total: 0.787803
60: 9(C) 11(C) Alpha: 0.542723 Beta: 0.542724 Total: 1.085447
61: 9(C) 15(C) Alpha: 0.545642 Beta: 0.545639 Total: 1.091281
62: 11(C) 12(H) Alpha: 0.435815 Beta: 0.435816 Total: 0.871630
63: 11(C) 13(H) Alpha: 0.432255 Beta: 0.432251 Total: 0.864506
64: 11(C) 14(H) Alpha: 0.450627 Beta: 0.450623 Total: 0.901250
65: 11(C) 15(C) Alpha: 0.046861 Beta: 0.046860 Total: 0.093721

66: 15(C) 16(H) Alpha: 0.449069 Beta: 0.449069 Total: 0.898138
67: 15(C) 17(H) Alpha: 0.428346 Beta: 0.428345 Total: 0.856691
68: 15(C) 18(H) Alpha: 0.435050 Beta: 0.435048 Total: 0.870099
69: 19(C) 20(H) Alpha: 0.399070 Beta: 0.399049 Total: 0.798118
70: 19(C) 21(C) Alpha: 0.544557 Beta: 0.544581 Total: 1.089139
71: 19(C) 25(C) Alpha: 0.542946 Beta: 0.542857 Total: 1.085804
72: 21(C) 22(H) Alpha: 0.434335 Beta: 0.434334 Total: 0.868669
73: 21(C) 23(H) Alpha: 0.449365 Beta: 0.449378 Total: 0.898743
74: 21(C) 24(H) Alpha: 0.437004 Beta: 0.437002 Total: 0.874005
75: 21(C) 25(C) Alpha: 0.045306 Beta: 0.045285 Total: 0.090591
76: 25(C) 26(H) Alpha: 0.427603 Beta: 0.427581 Total: 0.855184
77: 25(C) 27(H) Alpha: 0.429016 Beta: 0.428984 Total: 0.858000
78: 25(C) 28(H) Alpha: 0.448873 Beta: 0.448830 Total: 0.897703
79: 29(C) 30(C) Alpha: 0.548338 Beta: 0.548900 Total: 1.097238
80: 29(C) 31(C) Alpha: 0.045490 Beta: 0.044766 Total: 0.090257
81: 29(C) 32(C) Alpha: 0.045561 Beta: 0.045031 Total: 0.090593
82: 29(C) 33(C) Alpha: 0.557157 Beta: 0.556470 Total: 1.113626
83: 29(C) 34(C) Alpha: 0.553181 Beta: 0.552537 Total: 1.105718
84: 29(C) 38(C) Alpha: 0.028361 Beta: 0.028387 Total: 0.056748
85: 29(C) 50(C) Alpha: 0.028834 Beta: 0.028769 Total: 0.057603
86: 30(C) 31(C) Alpha: 0.560533 Beta: 0.559073 Total: 1.119606
87: 30(C) 32(C) Alpha: 0.044530 Beta: 0.044601 Total: 0.089131
88: 30(C) 33(C) Alpha: 0.044620 Beta: 0.044478 Total: 0.089098
89: 30(C) 34(C) Alpha: 0.028394 Beta: 0.028409 Total: 0.056803
90: 30(C) 38(C) Alpha: 0.556706 Beta: 0.556786 Total: 1.113492
91: 30(C) 41(H) Alpha: 0.025441 Beta: 0.025435 Total: 0.050876
92: 30(C) 42(C) Alpha: 0.028139 Beta: 0.028053 Total: 0.056191
93: 31(C) 32(C) Alpha: 0.557698 Beta: 0.557595 Total: 1.115293
94: 31(C) 33(C) Alpha: 0.044878 Beta: 0.044850 Total: 0.089728
95: 31(C) 38(C) Alpha: 0.029298 Beta: 0.029245 Total: 0.058543
96: 31(C) 42(C) Alpha: 0.557668 Beta: 0.557682 Total: 1.115350
97: 31(C) 43(H) Alpha: 0.025745 Beta: 0.025735 Total: 0.051480
98: 31(C) 46(C) Alpha: 0.028555 Beta: 0.028719 Total: 0.057274
99: 32(C) 33(C) Alpha: 0.560228 Beta: 0.559675 Total: 1.119903
100: 32(C) 42(C) Alpha: 0.029289 Beta: 0.029320 Total: 0.058609
101: 32(C) 46(C) Alpha: 0.556887 Beta: 0.556789 Total: 1.113676
102: 32(C) 50(C) Alpha: 0.029930 Beta: 0.029912 Total: 0.059843
103: 33(C) 34(C) Alpha: 0.027940 Beta: 0.027858 Total: 0.055799
104: 33(C) 46(C) Alpha: 0.027972 Beta: 0.027907 Total: 0.055879
105: 33(C) 50(C) Alpha: 0.554257 Beta: 0.554330 Total: 1.108587
106: 34(C) 35(H) Alpha: 0.443020 Beta: 0.442635 Total: 0.885654
107: 34(C) 36(H) Alpha: 0.435770 Beta: 0.435791 Total: 0.871561
108: 34(C) 37(H) Alpha: 0.429261 Beta: 0.429104 Total: 0.858364

109: 38(C) 39(H) Alpha: 0.430275 Beta: 0.430279 Total: 0.860554
110: 38(C) 40(H) Alpha: 0.438190 Beta: 0.438195 Total: 0.876385
111: 38(C) 41(H) Alpha: 0.441809 Beta: 0.441866 Total: 0.883674
112: 42(C) 43(H) Alpha: 0.441767 Beta: 0.441810 Total: 0.883577
113: 42(C) 44(H) Alpha: 0.437453 Beta: 0.437434 Total: 0.874887
114: 42(C) 45(H) Alpha: 0.424080 Beta: 0.424005 Total: 0.848085
115: 46(C) 47(H) Alpha: 0.432668 Beta: 0.432673 Total: 0.865342
116: 46(C) 48(H) Alpha: 0.442459 Beta: 0.442495 Total: 0.884954
117: 46(C) 49(H) Alpha: 0.419823 Beta: 0.419905 Total: 0.839728
118: 50(C) 51(H) Alpha: 0.442277 Beta: 0.442330 Total: 0.884607
119: 50(C) 52(H) Alpha: 0.435362 Beta: 0.435413 Total: 0.870775
120: 50(C) 53(H) Alpha: 0.435229 Beta: 0.435222 Total: 0.870451
121: 54(C) 55(C) Alpha: 0.520985 Beta: 0.520990 Total: 1.041975
122: 54(C) 58(C) Alpha: 0.044276 Beta: 0.044267 Total: 0.088544
123: 54(C) 68(C) Alpha: 0.035726 Beta: 0.035689 Total: 0.071415
124: 54(C) 78(C) Alpha: 0.034355 Beta: 0.034362 Total: 0.068717
125: 55(C) 56(H) Alpha: 0.408065 Beta: 0.408048 Total: 0.816113
126: 55(C) 57(H) Alpha: 0.413139 Beta: 0.413156 Total: 0.826295
127: 55(C) 58(C) Alpha: 0.544445 Beta: 0.544447 Total: 1.088892
128: 55(C) 61(C) Alpha: 0.038797 Beta: 0.038797 Total: 0.077594
129: 58(C) 59(H) Alpha: 0.420198 Beta: 0.420198 Total: 0.840396
130: 58(C) 60(H) Alpha: 0.416992 Beta: 0.416991 Total: 0.833982
131: 58(C) 61(C) Alpha: 0.561638 Beta: 0.561639 Total: 1.123277
132: 58(C) 64(C) Alpha: 0.041922 Beta: 0.041921 Total: 0.083843
133: 61(C) 62(H) Alpha: 0.430408 Beta: 0.430407 Total: 0.860815
134: 61(C) 63(H) Alpha: 0.433600 Beta: 0.433600 Total: 0.867200
135: 61(C) 64(C) Alpha: 0.583784 Beta: 0.583784 Total: 1.167569
136: 64(C) 65(H) Alpha: 0.450908 Beta: 0.450908 Total: 0.901816
137: 64(C) 66(H) Alpha: 0.455293 Beta: 0.455294 Total: 0.910587
138: 64(C) 67(H) Alpha: 0.447275 Beta: 0.447275 Total: 0.894550
139: 68(C) 69(H) Alpha: 0.395379 Beta: 0.395377 Total: 0.790756
140: 68(C) 70(C) Alpha: 0.540410 Beta: 0.540443 Total: 1.080852
141: 68(C) 74(C) Alpha: 0.544473 Beta: 0.544447 Total: 1.088920
142: 70(C) 71(H) Alpha: 0.432002 Beta: 0.432044 Total: 0.864045
143: 70(C) 72(H) Alpha: 0.450045 Beta: 0.450011 Total: 0.900056
144: 70(C) 73(H) Alpha: 0.437363 Beta: 0.437201 Total: 0.874563
145: 70(C) 74(C) Alpha: 0.045615 Beta: 0.045595 Total: 0.091210
146: 74(C) 75(H) Alpha: 0.440510 Beta: 0.440508 Total: 0.881018
147: 74(C) 76(H) Alpha: 0.451767 Beta: 0.451755 Total: 0.903522
148: 74(C) 77(H) Alpha: 0.432741 Beta: 0.432741 Total: 0.865483
149: 78(C) 79(H) Alpha: 0.397262 Beta: 0.397271 Total: 0.794533
150: 78(C) 80(C) Alpha: 0.538944 Beta: 0.538957 Total: 1.077901
151: 78(C) 84(C) Alpha: 0.542705 Beta: 0.542662 Total: 1.085367

152: 80(C) 81(H) Alpha: 0.443671 Beta: 0.443675 Total: 0.887346
153: 80(C) 82(H) Alpha: 0.424637 Beta: 0.424621 Total: 0.849258
154: 80(C) 83(H) Alpha: 0.424275 Beta: 0.424288 Total: 0.848563
155: 80(C) 84(C) Alpha: 0.044481 Beta: 0.044469 Total: 0.088950
156: 84(C) 85(H) Alpha: 0.437834 Beta: 0.437838 Total: 0.875672
157: 84(C) 86(H) Alpha: 0.449973 Beta: 0.449961 Total: 0.899934
158: 84(C) 87(H) Alpha: 0.436870 Beta: 0.436870 Total: 0.873740
159: 88(C) 89(C) Alpha: 0.557380 Beta: 0.557513 Total: 1.114892
160: 88(C) 90(C) Alpha: 0.044750 Beta: 0.044624 Total: 0.089374
161: 88(C) 91(C) Alpha: 0.045496 Beta: 0.044801 Total: 0.090297
162: 88(C) 92(C) Alpha: 0.557331 Beta: 0.556605 Total: 1.113936
163: 88(C) 93(C) Alpha: 0.553327 Beta: 0.553059 Total: 1.106386
164: 88(C) 97(C) Alpha: 0.027899 Beta: 0.028018 Total: 0.055917
165: 88(C) 109(C) Alpha: 0.028198 Beta: 0.028163 Total: 0.056361
166: 89(C) 90(C) Alpha: 0.557826 Beta: 0.557337 Total: 1.115162
167: 89(C) 91(C) Alpha: 0.045272 Beta: 0.045245 Total: 0.090517
168: 89(C) 92(C) Alpha: 0.044785 Beta: 0.044836 Total: 0.089620
169: 89(C) 93(C) Alpha: 0.029349 Beta: 0.029368 Total: 0.058717
170: 89(C) 97(C) Alpha: 0.555180 Beta: 0.555070 Total: 1.110251
171: 89(C) 98(H) Alpha: 0.025278 Beta: 0.025275 Total: 0.050553
172: 89(C) 101(C) Alpha: 0.028567 Beta: 0.028533 Total: 0.057100
173: 90(C) 91(C) Alpha: 0.560356 Beta: 0.560012 Total: 1.120368
174: 90(C) 92(C) Alpha: 0.045091 Beta: 0.045078 Total: 0.090169
175: 90(C) 97(C) Alpha: 0.027987 Beta: 0.027921 Total: 0.055909
176: 90(C) 101(C) Alpha: 0.556950 Beta: 0.557039 Total: 1.113988
177: 90(C) 105(C) Alpha: 0.029093 Beta: 0.029068 Total: 0.058161
178: 91(C) 92(C) Alpha: 0.552477 Beta: 0.552421 Total: 1.104898
179: 91(C) 101(C) Alpha: 0.027963 Beta: 0.028101 Total: 0.056064
180: 91(C) 105(C) Alpha: 0.558107 Beta: 0.557856 Total: 1.115964
181: 91(C) 107(H) Alpha: 0.025261 Beta: 0.025287 Total: 0.050548
182: 91(C) 109(C) Alpha: 0.028603 Beta: 0.028609 Total: 0.057212
183: 92(C) 93(C) Alpha: 0.028387 Beta: 0.028338 Total: 0.056725
184: 92(C) 105(C) Alpha: 0.028459 Beta: 0.028453 Total: 0.056912
185: 92(C) 109(C) Alpha: 0.551393 Beta: 0.551508 Total: 1.102901
186: 93(C) 94(H) Alpha: 0.435244 Beta: 0.435253 Total: 0.870497
187: 93(C) 95(H) Alpha: 0.442517 Beta: 0.442477 Total: 0.884994
188: 93(C) 96(H) Alpha: 0.435159 Beta: 0.435168 Total: 0.870327
189: 97(C) 98(H) Alpha: 0.443184 Beta: 0.443228 Total: 0.886412
190: 97(C) 99(H) Alpha: 0.436711 Beta: 0.436736 Total: 0.873447
191: 97(C) 100(H) Alpha: 0.428677 Beta: 0.428776 Total: 0.857453
192: 101(C) 102(H) Alpha: 0.418989 Beta: 0.418554 Total: 0.837543
193: 101(C) 103(H) Alpha: 0.427355 Beta: 0.427333 Total: 0.854689
194: 101(C) 104(H) Alpha: 0.441888 Beta: 0.441291 Total: 0.883179

195: 105(C) 106(H) Alpha: 0.430937 Beta: 0.430864 Total: 0.861800
196: 105(C) 107(H) Alpha: 0.442473 Beta: 0.442265 Total: 0.884739
197: 105(C) 108(H) Alpha: 0.437272 Beta: 0.437278 Total: 0.874550
198: 109(C) 110(H) Alpha: 0.444183 Beta: 0.444248 Total: 0.888432
199: 109(C) 111(H) Alpha: 0.431994 Beta: 0.432023 Total: 0.864018
200: 109(C) 112(H) Alpha: 0.436142 Beta: 0.436144 Total: 0.872286
201: 113(C) 114(H) Alpha: 0.418089 Beta: 0.418088 Total: 0.836177
202: 113(C) 115(H) Alpha: 0.417288 Beta: 0.417285 Total: 0.834573
203: 113(C) 116(C) Alpha: 0.041375 Beta: 0.041375 Total: 0.082750
204: 113(C) 120(C) Alpha: 0.545280 Beta: 0.545216 Total: 1.090497
205: 113(C) 123(C) Alpha: 0.559461 Beta: 0.559425 Total: 1.118885
206: 116(C) 117(H) Alpha: 0.449040 Beta: 0.449040 Total: 0.898080
207: 116(C) 118(H) Alpha: 0.445872 Beta: 0.445870 Total: 0.891742
208: 116(C) 119(H) Alpha: 0.455441 Beta: 0.455439 Total: 0.910880
209: 116(C) 123(C) Alpha: 0.584617 Beta: 0.584617 Total: 1.169234
210: 120(C) 121(H) Alpha: 0.411943 Beta: 0.411827 Total: 0.823770
211: 120(C) 122(H) Alpha: 0.403975 Beta: 0.403968 Total: 0.807944
212: 120(C) 123(C) Alpha: 0.040165 Beta: 0.040174 Total: 0.080339
213: 123(C) 124(H) Alpha: 0.433371 Beta: 0.433364 Total: 0.866736
214: 123(C) 125(H) Alpha: 0.430223 Beta: 0.430219 Total: 0.860442
215: 126(N) 127(C) Alpha: 0.578061 Beta: 0.554013 Total: 1.132074
216: 126(N) 128(H) Alpha: 0.031619 Beta: 0.026914 Total: 0.058533
217: 126(N) 130(H) Alpha: 0.028445 Beta: 0.026891 Total: 0.055335
218: 127(C) 128(H) Alpha: 0.433500 Beta: 0.421729 Total: 0.855229
219: 127(C) 129(H) Alpha: 0.421815 Beta: 0.421175 Total: 0.842990
220: 127(C) 130(H) Alpha: 0.435098 Beta: 0.431814 Total: 0.866911

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