

Supplementary Information

Azole-containing cationic bis-cyclometallated iridium(III) isocyanide complexes: a theoretical insight on the emission energy and emission efficiency

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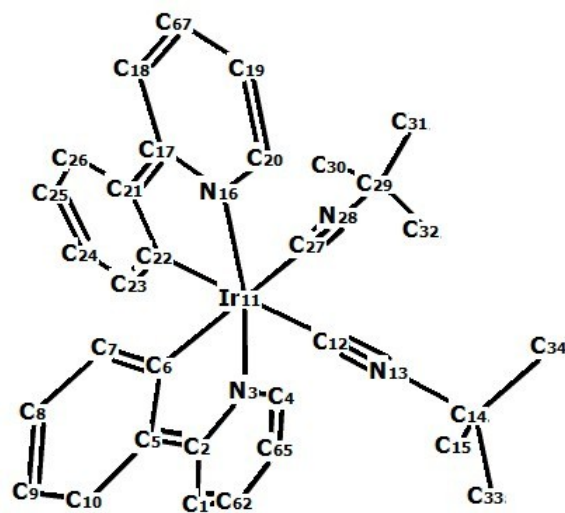


Figure S1. Atom labelling used for the studied complexes, exemplified for the **A1** molecule.

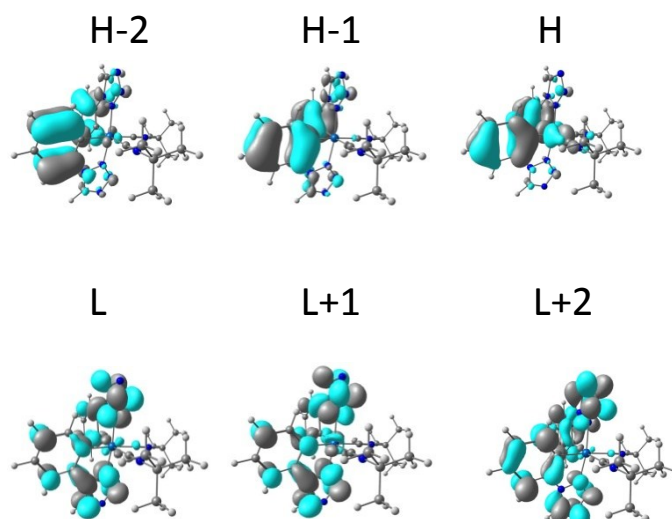


Figure S2. Frontier orbitals (isovalue contour plots ± 0.03 a.u.), exemplified for the **N4** complex at its optimized ground-state geometry. H and L denote HOMO and LUMO, respectively.

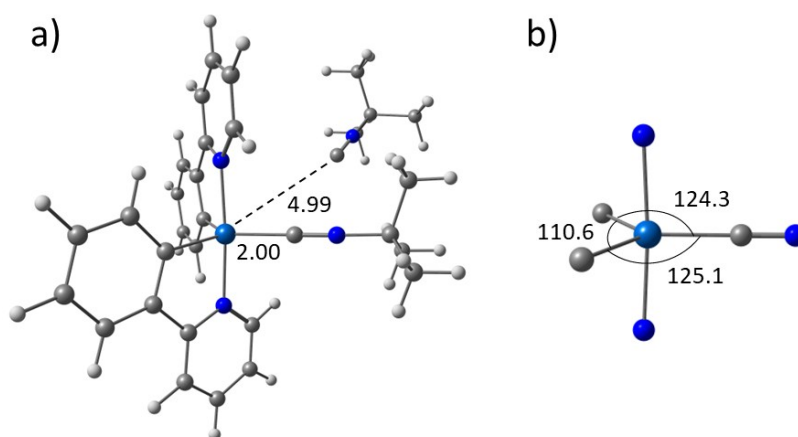


Figure S3. a) Minimum-energy optimized structure calculated for the ^3MC state of complex **A1**. Ir \cdots C distances (in Å) are indicated for the CN-*tert*-Bu ligands. b) Metal coordination sphere calculated for the ^3MC state of complex **A1** highlighting the trigonal bipyramidal coordination of the Ir(III) atom. Selected angles are reported in degrees.

Table S1. Selected bond distances (in Å), angles (degrees), and dihedral angles (degrees) for complexes **A1**, **N2-N4** and **C2-C4** at their corresponding ground-state optimized geometry. The atom labelling reported in Figure S1 has been used to define the distances, angles and dihedrals.

	A1	N2	N3	N4	C2	C3	C4
	Distances (Å)						
Ir ₁₁ -N ₃	2.097	2.064	2.050	2.043	2.075	2.059	2.055
Ir ₁₁ -C ₆	2.073	2.083	2.084	2.087	2.097	2.098	2.103
Ir ₁₁ -N ₁₆	2.097	2.064	2.050	2.043	2.075	2.060	2.055
Ir ₁₁ -C ₂₇	2.042	2.040	2.044	2.050	2.032	2.036	2.040
Ir ₁₁ -C ₁₂	2.042	2.040	2.044	2.050	2.032	2.037	2.040
Ir ₁₁ -C ₂₂	2.074	2.083	2.084	2.087	2.097	2.098	2.103
	Angles (degrees)						
N ₃ -Ir ₁₁ -C ₆	79.42	78.95	78.77	78.72	79.13	78.71	78.49
C ₆ -Ir ₁₁ -N ₁₆	93.79	93.61	93.96	94.21	93.27	93.32	93.36
N ₁₆ -Ir ₁₁ -C ₂₇	89.48	91.23	91.69	91.59	91.27	91.87	91.96
C ₂₇ -Ir ₁₁ -N ₃	96.93	95.76	95.22	95.17	95.88	95.70	95.77
N ₃ -Ir ₁₁ -C ₂₂	96.86	93.70	93.95	94.22	93.28	93.32	93.34
C ₂₂ -Ir ₁₁ -N ₁₆	79.43	78.96	78.77	78.73	79.12	78.71	78.49
N ₁₆ -Ir ₁₁ -C ₁₂	93.76	95.89	95.25	95.16	95.88	95.75	95.80
C ₁₂ -Ir ₁₁ -N ₃	89.57	91.07	91.70	91.57	91.27	91.83	91.96
C ₁₂ -Ir ₁₁ -C ₆	89.72	90.07	89.96	89.85	89.69	89.74	89.88
C ₆ -Ir ₁₁ -C ₂₂	87.45	87.58	88.12	88.36	87.47	88.10	87.86
C ₂₂ -Ir ₁₁ -C ₂₇	89.73	89.57	89.82	89.95	89.58	89.64	89.89
C ₂₇ -Ir ₁₁ -C ₁₂	93.35	93.25	92.73	92.50	93.70	93.05	92.95
	Dihedrals (degrees)						
N ₃ -C ₂ (N ₂)-C ₅ -C ₆	0.073	-0.114	-0.05	-0.355	0.147	0.200	-0.229
N ₁₆ -C ₁₇ (N ₁₇)-C ₂₁ -C ₂₂	0.042	-0.476	-0.011	-0.298	0.190	0.137	-0.219

Table S2. Cartesian coordinates (x, y, z , in Å) of the S_0 , T_1 and 3MC optimized structures for the studied complexes. All calculations performed at the B3LYP/(6-31G**+LANL2DZ) level in the presence of solvent (acetonitrile).

A1 – State S_0

C 2.655664 -1.443123 -3.108929
C 1.960479 -1.242511 -1.907439
N 0.978662 -0.292295 -1.848582
C 0.691003 0.449151 -2.937944
C 2.194542 -1.973992 -0.659682
C 1.376484 -1.603856 0.436879
C 1.580476 -2.270986 1.651593
C 2.549136 -3.270253 1.778341
C 3.344899 -3.628498 0.685258
C 3.168804 -2.979861 -0.532314
Ir 0.001548 -0.114945 -0.001300
C 1.364011 1.296203 0.566364
N 2.166702 2.080809 0.886876
C 3.173117 3.052939 1.278145
C 4.006015 2.434004 2.413990
N -0.974567 -0.279108 1.847917
C -1.945599 -1.239578 1.918633
C -2.639072 -1.432574 3.122359
C -1.355435 0.324270 4.136437
C -0.696583 0.480158 2.927529
C -2.171631 -1.988986 0.680026
C -1.358473 -1.622744 -0.421463
C -1.556378 -2.305671 -1.628368
C -2.514021 -3.316978 -1.742655
C -3.304515 -3.671696 -0.644601
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C -1.375538 1.276347 -0.583613
N -2.187878 2.048821 -0.909230
C -3.208926 3.004685 -1.302507
C -4.348269 2.221129 -1.977075
C -3.698915 3.713572 -0.027697
C -2.565725 4.002927 -2.280692
C 4.045242 3.342461 0.043825
C 2.441556 4.320919 1.750915
H 4.096722 -4.405393 0.783504
H 3.791810 -3.261207 -1.375655
H 0.979778 -2.014823 2.519404
H 2.684842 -3.771998 2.732851
H -0.959370 -2.052788 -2.499689
H -3.753536 -3.285949 1.412452
H -2.645174 -3.831003 -2.691250
H -4.047572 -4.458138 -0.733097
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H 3.181066 5.068983 2.047937
H 4.496266 1.515599 2.080992
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H 4.810490 4.075123 0.312778
H 4.541208 2.432920 -0.304658
H 3.442903 3.752095 -0.771238
H -1.737453 4.535549 -1.806335
H -2.193849 3.490613 -3.171862
H -3.317676 4.733713 -2.589225
H -4.781167 1.492388 -1.286928
H -5.131330 2.920547 -2.281188

H -3.986683 1.696315 -2.865158
H -4.465396 4.444150 -0.298815
H -4.133829 2.996838 0.673678
H -2.877210 4.238624 0.466310
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H 3.431968 -2.196185 -3.157026
H 2.892444 -0.842272 -5.157990
C 1.351152 0.285267 -4.145082
H 1.081466 0.904737 -4.991912
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H 0.076628 1.226139 2.801939
H -1.093727 0.958054 4.975139
H -2.883801 -0.808125 5.163409
H -3.406882 -2.193649 3.179832

N2 – State S₀

C 1.001589 -0.338152 -4.177405
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N 1.537122 -1.216173 -2.217922
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C 2.049451 -1.920378 -1.092079
C 1.473347 -1.565678 0.142080
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H -4.584545 2.289191 0.882838
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H 1.824515 4.573648 1.544944
H 2.498980 3.516593 2.806504
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H 4.296282 1.800583 2.210964
H 4.330108 4.612961 -0.324005
H 3.903910 3.180409 -1.280767
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N3 – State S₀

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N4 – State S₀

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C -2.615972 4.332038 -1.311505
C -4.247580 2.467940 -1.876937

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C 4.535674 2.317588 1.319446
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H -2.347439 -1.806840 4.121008

C2 – State S_0

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N 2.176399 -0.308286 -3.650115
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C3 – State S_0

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C 1.401229 -1.664040 0.325622
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C 2.657228 -3.357689 1.556445
C 3.376037 -3.705339 0.409138
C 3.122671 -3.038482 -0.787610
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C 1.387170 1.243928 0.561909
N 2.186174 2.020953 0.906374
C 3.171820 2.991300 1.348229
C 3.940826 2.373478 2.528946
C 1.439065 0.272594 -5.262159

N -0.845580 -0.351103 1.866095
C -1.839789 -1.286147 1.988103
C -2.224067 -1.247090 3.315079
N -1.435609 -0.299251 3.885039
N -0.595539 0.249554 3.005375
C -1.429178 0.152226 5.274510
C -2.190130 -2.007053 0.773733
C -1.433189 -1.625514 -0.366075
C -1.729687 -2.276005 -1.569540
C -2.721219 -3.261443 -1.641185
C -3.449603 -3.622891 -0.504227
C -3.184865 -2.991971 0.709406
C -1.360914 1.284124 -0.526089
N -2.146305 2.082314 -0.853039
C -3.114034 3.077882 -1.278134
C -4.213008 2.353193 -2.074644
C -3.690180 3.740422 -0.014693
C -2.373453 4.102675 -2.155413
C 4.110588 3.277156 0.163115
C 2.417223 4.261244 1.778576
H 4.128518 -4.487009 0.447791
H 3.678735 -3.298541 -1.684401
H 1.150561 -2.102373 2.423749
H 2.854515 -3.872969 2.492874
H 2.380566 0.787367 -5.460866
H 1.319516 -0.563164 -5.952306
H 0.606447 0.965210 -5.368347
H -1.186592 -2.017039 -2.474097
H -3.747266 -3.263572 1.598817
H -2.926964 -3.748865 -2.590619
H -4.217946 -4.387630 -0.563831
H -0.625030 0.877614 5.381007
H -1.253934 -0.698910 5.933707
H -2.386311 0.617824 5.514564
H 1.846022 4.676084 0.943948
H 1.732891 4.046466 2.603417
H 3.139901 5.010489 2.111862
H 4.448492 1.454735 2.224043
H 4.692041 3.086604 2.878429
H 3.264819 2.146234 3.357257
H 4.861246 4.009230 0.471693
H 4.623493 2.366048 -0.155822
H 3.554504 3.685368 -0.684887
H -1.578224 4.596208 -1.590560
H -1.935954 3.619653 -3.032958
H -3.082213 4.862755 -2.494104
H -4.712609 1.604559 -1.454327
H -4.956305 3.083549 -2.404770
H -3.794583 1.859885 -2.955718
H -4.420557 4.497980 -0.310570
H -4.191392 3.002521 0.617114
H -2.901013 4.225468 0.565534
H 2.919207 -1.757363 -3.924168
H -2.962919 -1.795209 3.876501

C4 – State S_0

C -3.356472 -3.679583 -0.644461
C -3.179608 -3.022092 0.569056
C -2.207027 -2.018300 0.664096
C -1.385301 -1.638778 -0.429425
C -1.597418 -2.317659 -1.634945
C -2.565154 -3.322719 -1.741831

H -4.104145 -4.460680 -0.738037
H -3.784263 -3.278708 1.433879
H -1.008491 -2.067874 -2.512560
H -2.704349 -3.832055 -2.691607
C -1.942348 -1.262684 1.871652
N -0.962444 -0.314856 1.804124
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N -1.769352 -0.319259 3.715463
C -1.992482 0.038672 5.112045
H -3.027489 0.358958 5.233208
H -1.792653 -0.831363 5.738019
H -1.310293 0.849830 5.356379
C 1.399321 -1.623012 0.440933
C 2.225233 -2.003765 -0.648973
C 1.615998 -2.291190 1.651627
C 3.206577 -2.998147 -0.545451
C 2.592462 -3.286810 1.767023
H 1.023882 -2.040291 2.526757
C 3.388118 -3.644822 0.673175
H 3.814198 -3.256051 -1.407811
H 2.735080 -3.787798 2.720725
H 4.142641 -4.418476 0.773370
C 1.954442 -1.260354 -1.862706
N 0.965703 -0.321167 -1.803558
N 2.480215 -1.277334 -3.084205
N 0.859021 0.259734 -2.977258
N 1.774173 -0.333563 -3.714205
C 1.995001 0.014793 -5.113561
H 1.304973 0.816970 -5.365410
H 1.804434 -0.862505 -5.732240
H 3.026872 0.344343 -5.236600
Ir 0.000428 -0.116657 -0.000625
C -1.340914 1.279600 -0.642330
C 1.329118 1.296506 0.630145
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N 2.089823 2.087439 1.022275
C -3.057121 3.035578 -1.551800
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C -3.788485 2.392420 -2.742806
C -4.036569 3.374842 -0.414888
H -1.717757 4.709164 -1.145248
H -1.544023 4.020678 -2.776093
H -2.952187 5.025649 -2.380594
H -4.327140 1.494432 -2.429520
H -4.509685 3.107967 -3.146051
H -3.083642 2.125124 -3.534264
H -4.759924 4.110115 -0.776521
H -4.579541 2.483610 -0.089690
H -3.507390 3.799643 0.442032
C 3.029716 3.071445 1.532066
C 2.233923 4.076442 2.382910
C 4.073167 2.323874 2.380313
C 3.685294 3.760688 0.322960
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H 1.741500 3.574691 3.219862
H 2.920419 4.827144 2.782694
H 4.610383 1.587908 1.776581
H 4.795045 3.043888 2.774367
H 3.598045 1.812271 3.221304
H 4.398375 4.507458 0.681798
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A1 – State T₁

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C 1.997359 -1.219762 -1.897037
N 1.009528 -0.275713 -1.848016
C 0.738755 0.476352 -2.933926
C 1.423432 0.329321 -4.129739
C 2.432550 -0.633393 -4.204838
C 2.212541 -1.962482 -0.651596
C 3.189288 -2.964819 -0.516063
C 3.346822 -3.624298 0.698424
C 2.530560 -3.280972 1.781096
C 1.559745 -2.284651 1.647258
C 1.374717 -1.608504 0.435287
Ir -0.000774 -0.124293 -0.009336
C -1.375180 1.292385 -0.580348
N -2.172985 2.080012 -0.903740
C -3.172789 3.056777 -1.301678
C -4.056349 3.344421 -0.075165
C 1.353900 1.288192 0.596603
N 2.149595 2.070764 0.937011
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C 3.869792 3.546336 0.102463
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C -1.997378 -1.296885 1.853329
C -2.199949 -1.988267 0.663881
C -1.335226 -1.609661 -0.484732
C -1.515817 -2.281628 -1.681098
C -2.482038 -3.295003 -1.827244
C -3.311645 -3.660099 -0.719177
C -3.187547 -3.037676 0.489776
C 2.409491 4.183285 2.079776
C 4.119650 2.320585 2.312409
C -2.431993 4.323694 -1.762770
C -3.995540 2.443488 -2.447907
H -4.050905 -4.445331 -0.848124
H -3.826275 -3.328352 1.316007
H -0.902193 -2.027466 -2.540280
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H 0.940618 -2.037684 2.504538
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H 2.651783 -3.792120 2.732535
H 4.100667 -4.398511 0.802257
H -1.823523 4.735758 -0.953558
H -1.785409 4.108197 -2.617387
H -3.166064 5.075684 -2.063236
H -4.492239 1.525788 -2.122644
H -4.759106 3.160048 -2.761374
H -3.358788 2.216441 -3.306842
H -4.816570 4.080248 -0.349578
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H -3.461247 3.749422 0.747470
H 1.696993 4.669280 1.408289
H 1.873042 3.811303 2.956609
H 3.140278 4.926460 2.408910
H 4.618574 1.490885 1.805026
H 4.879986 3.030532 2.647972
H 3.593594 1.934471 3.189336
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H 3.168705 4.033672 -0.580033
H -0.050169 1.208584 -2.824260

H 1.167307 0.956303 -4.975245
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H 3.499187 -2.151395 -3.127781
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C -2.445299 -0.750231 4.195358
C -0.742513 0.424995 2.913962
C -1.432745 0.248010 4.117530
H -2.989982 -0.908425 5.119424
H -1.183152 0.873024 4.965916
H 0.031771 1.179374 2.837112
H -3.483061 -2.266240 3.117538

N2 – State T₁

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N 0.596279 -0.317055 -1.943110
C 0.371385 0.262772 -3.149752
C 1.135806 -0.366970 -4.142972
C 1.943201 -2.047949 -1.111924
C 1.356947 -1.662829 0.200246
C 1.783654 -2.381055 1.293021
C 2.729808 -3.432916 1.176809
C 3.275036 -3.789396 -0.106253
C 2.907790 -3.129399 -1.238494
Ir 0.007126 -0.119787 0.020370
C 1.489668 1.247173 0.363364
N 2.339771 2.016099 0.577745
C 3.395507 2.978030 0.845330
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C -1.102005 -0.317928 4.175297
C -0.298991 0.247707 3.173565
C -2.118634 -1.877071 1.067991
C -1.501695 -1.547088 -0.152874
C -1.977363 -2.209265 -1.289523
C -3.009620 -3.150513 -1.207117
C -3.596273 -3.449492 0.024682
C -3.152080 -2.808160 1.180800
C -1.375169 1.340126 -0.346145
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C -3.188210 3.152884 -0.880554
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C -3.617278 3.795215 0.450157
C -2.548495 4.190483 -1.819384
C 4.147022 3.223641 -0.474671
C 2.732054 4.268615 1.356408
H -1.084806 -0.099378 5.231291
H 1.151623 -0.117534 -5.193015
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H 3.313267 -3.397166 -2.206674
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H 3.049032 -3.978183 2.058260
H -1.538476 -1.987753 -2.258031
H -3.607362 -3.034301 2.139383
H -3.357747 -3.650254 -2.106629
H -4.398412 -4.177556 0.090675
H 2.053873 4.681992 0.605386
H 2.170552 4.080670 2.275287
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H 4.588968 2.296977 -0.849723
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H -3.289126 4.957462 -2.060037
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H -5.144132 3.175442 -1.791600
H -4.052414 1.964140 -2.492843
H -4.374100 4.557767 0.249494
H -4.046159 3.048020 1.122851
H -2.766987 4.271252 0.945328
H -2.691822 -1.877927 3.901849
H 2.574130 -2.082972 -3.905648
H -0.322512 1.084580 -3.232474
H 0.476614 0.994340 3.245859

N3 – State T₁

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C 1.917445 -1.174936 -3.522073
N 1.638927 -1.169248 -2.198468
N 0.616128 -0.309660 -1.977203
N 0.232434 0.231273 -3.102239
C 2.178784 -1.841358 -1.062184
C 1.558319 -1.518614 0.158169
C 2.068244 -2.152248 1.296349
C 3.130883 -3.057525 1.208710
C 3.717347 -3.350144 -0.025867
C 3.241813 -2.736576 -1.183315
Ir 0.002878 -0.143011 -0.018558
C 1.339174 1.369797 0.326577
N 2.108812 2.213531 0.552436
C 3.065548 3.265282 0.854453
C 3.524003 3.875687 -0.481189
H 0.899724 0.006078 -5.110643
C -1.316724 -1.712373 -0.163276
C -1.910468 -2.084312 1.150484
C -2.860590 -3.162713 1.286453
C -3.209229 -3.849599 0.162330
C -2.654079 -3.512463 -1.122439
C -1.727393 -2.460975 -1.251168
N -1.506116 -1.349040 2.183787
N -0.550847 -0.326577 1.940221
N -0.317780 0.335551 3.065748
C -1.072795 -0.255781 4.038136
C -1.817857 -1.296494 3.549834
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C -1.516573 1.191780 -0.367522
N -2.378181 1.943498 -0.587935
C -3.445034 2.888300 -0.874366
C -4.217839 3.127624 0.434195
C -2.792488 4.185588 -1.382239
C -4.349075 2.260421 -1.949103
C 2.348226 4.308847 1.728419
C 4.242843 2.620989 1.606428
H -3.919027 -4.667741 0.230031
H -3.273797 -3.412859 2.256096
H -1.336817 -2.232732 -2.237884
H -2.961789 -4.078626 -1.994592
H 1.633828 -1.936350 2.267812

H 3.693334 -2.953523 -2.145592
H 3.505552 -3.536066 2.108880
H 4.543000 -4.050997 -0.090742
H -2.132126 4.612731 -0.623162
H -2.214624 4.000854 -2.291441
H -3.576500 4.912236 -1.610314
H -4.783048 1.322237 -1.593919
H -5.161551 2.954559 -2.178658
H -3.787413 2.066428 -2.866408
H -5.028300 3.835864 0.243613
H -4.650918 2.195954 0.807156
H -3.562955 3.546721 1.202395
H 1.495191 4.740845 1.198835
H 1.996334 3.860199 2.660862
H 3.049772 5.111151 1.970775
H 4.723422 1.854469 0.993115
H 4.980343 3.393239 1.839621
H 3.905961 2.166798 2.541725
H 4.242073 4.674180 -0.278018
H 4.008963 3.122733 -1.107773
H 2.677661 4.299835 -1.027580
H 2.693891 -1.783775 -3.953937
H -2.517272 -1.973314 4.007739

N4 – State T₁

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N 0.554137 -0.336894 -1.934893
N 0.382375 0.348488 -3.067248
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C 1.294290 -1.738190 0.163323
C 1.689383 -2.502506 1.250983
C 2.608912 -3.551850 1.118656
C 3.177500 -3.875848 -0.166555
C 2.845158 -3.174436 -1.288682
Ir -0.008152 -0.156363 0.018499
C 1.526454 1.163872 0.383333
N 2.394489 1.904192 0.610335
C 3.477943 2.829229 0.904869
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C -1.592965 -1.500763 -0.177611
C -2.233309 -1.815791 1.033659
C -3.313963 -2.689794 1.149519
C -3.790950 -3.289300 -0.013687
C -3.188245 -3.003032 -1.242606
C -2.107069 -2.119640 -1.321790
N -1.687410 -1.153906 2.174228
N -0.641199 -0.321105 1.967407
N -0.281843 0.193066 3.106799
N -1.076779 -0.287251 4.074721
C -1.939121 -1.113842 3.493760
C -1.318028 1.386874 -0.331453
N -2.066489 2.247956 -0.556365
C -2.998020 3.325707 -0.851438
C -3.719644 3.685866 0.458597
C -2.178186 4.513697 -1.383637
C -3.985842 2.807829 -1.910899
C 2.965654 3.820790 1.963504
C 4.661150 2.003153 1.437956
H -4.630014 -3.974491 0.041102
H -3.773946 -2.900356 2.109093

H -1.662784 -1.911238 -2.290094
H -3.565540 -3.471136 -2.146907
H 1.290552 -2.283808 2.236136
H 3.269107 -3.415755 -2.255788
H 2.906516 -4.131207 1.985348
H 3.884263 -4.696222 -0.235285
H -1.454488 4.853383 -0.638364
H -1.645285 4.241029 -2.298015
H -2.858059 5.339057 -1.609547
H -4.540055 1.942994 -1.537584
H -4.698032 3.602189 -2.148071
H -3.461768 2.524885 -2.827237
H -4.424111 4.497889 0.262081
H -4.276020 2.828516 0.845886
H -3.007383 4.019210 1.217596
H 2.105203 4.380965 1.588899
H 2.677782 3.298837 2.879563
H 3.764499 4.527589 2.201722
H 4.995833 1.275972 0.693764
H 5.491093 2.677982 1.662246
H 4.385799 1.473491 2.353452
H 4.659414 4.247603 -0.209111
H 4.172039 2.833366 -1.163901
H 2.989257 4.109355 -0.793406
H 2.514992 -1.850725 -4.050638
H -2.719200 -1.670902 3.986621

C2 – State T₁

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C 2.259661 -2.007726 -0.447161
C 1.312942 -1.648194 0.548613
C 1.365478 -2.346477 1.760418
C 2.307004 -3.359212 1.981325
C 3.228636 -3.697875 0.987006
C 3.205516 -3.019443 -0.230515
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C 1.280266 1.248664 0.796650
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C 2.950347 2.931372 1.911288
C 4.325346 2.734684 1.249210
C 2.573635 0.159089 -5.007767
C -1.311754 -1.593601 -0.659261
C -2.301670 -1.980814 0.400732
C -3.303440 -3.021093 0.126767
C -3.319947 -3.622279 -1.094270
C -2.377334 -3.255760 -2.114001
C -1.395028 -2.244165 -1.861583
C -2.187705 -1.301994 1.590923
N -1.166112 -0.322657 1.689771
C -1.230385 0.209141 2.889547
N -2.231265 -0.344376 3.625589
C -2.863146 -1.300798 2.854105
C -2.576769 0.008832 4.997522
C -1.255560 1.313760 -0.745410
N -1.979487 2.113830 -1.193194
C -2.879020 3.102676 -1.758997
C -3.992465 3.365481 -0.729981
C -2.063063 4.378352 -2.031634

C -3.454764 2.522771 -3.062811
C 2.420240 4.356743 1.677098
C 3.005197 2.600122 3.413108
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H -2.413397 -3.749821 -3.079562
H -3.611342 0.356786 5.042846
H -2.458732 -0.860695 5.648414
H -1.914765 0.804845 5.336898
H 0.662288 -2.105212 2.552909
H 3.920159 -3.275732 -1.008753
H 2.320832 -3.884757 2.932886
H 3.959245 -4.482861 1.158864
H 1.926235 0.973906 -5.329977
H 2.447368 -0.690087 -5.682140
H 3.612662 0.493041 -5.033654
H -1.635314 4.772359 -1.106033
H -1.252807 4.178659 -2.737838
H -2.719771 5.138521 -2.462611
H -4.008120 1.600452 -2.867674
H -4.137959 3.251140 -3.507327
H -2.657820 2.310894 -3.780529
H -4.685764 4.107935 -1.133906
H -4.549231 2.449207 -0.517430
H -3.575519 3.751045 0.204046
H 2.355644 4.577702 0.608481
H 1.430800 4.483010 2.124432
H 3.104063 5.073347 2.139478
H 3.357980 1.578038 3.573578
H 3.696302 3.288421 3.906602
H 2.019019 2.709401 3.872439
H 5.044041 3.420031 1.705943
H 4.681819 1.711118 1.390449
H 4.274850 2.946782 0.178036
H -3.691755 -1.880469 3.224048
H 3.635359 -1.793852 -3.281933
H 0.579672 1.117231 -3.248736
H -0.584375 0.985377 3.271523

C3 – State T₁

N 1.599172 -0.197611 -3.837781
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C 1.905231 -1.248295 -1.956964
N 0.918574 -0.303630 -1.849762
N 0.727250 0.335067 -2.979464
C 2.196677 -2.008003 -0.750351
C 1.398843 -1.650183 0.368678
C 1.640298 -2.334387 1.565155
C 2.617874 -3.332891 1.649138
C 3.387682 -3.671252 0.532587
C 3.178776 -3.004468 -0.672871
Ir -0.002714 -0.136448 -0.012872
C 1.355594 1.254007 0.611995
N 2.142948 2.027371 0.989713
C 3.118139 2.986679 1.476798
C 4.409715 2.794157 0.663178
C 1.654623 0.290392 -5.213686
C -1.381300 -1.624459 -0.465927
C -2.216032 -2.023934 0.735786
C -3.233847 -3.068715 0.611127
C -3.419185 -3.667692 -0.590936

C -2.630900 -3.291925 -1.750988
C -1.634927 -2.277682 -1.644084
C -1.922922 -1.324324 1.894508
N -0.909632 -0.353358 1.818512
N -0.724950 0.244898 2.967400
N -1.598916 -0.313763 3.819083
C -2.356886 -1.270006 3.241364
C -1.636784 0.144287 5.205707
C -1.358849 1.287493 -0.573327
N -2.135908 2.085577 -0.919377
C -3.098459 3.077770 -1.364144
C -4.049928 3.365447 -0.189673
C -2.316356 4.339653 -1.768162
C -3.859684 2.486417 -2.563340
C 2.534338 4.394936 1.268718
C 3.353160 2.696431 2.969519
H -4.170432 -4.445049 -0.699982
H -3.824239 -3.349716 1.477693
H -1.068769 -2.024422 -2.536605
H -2.808953 -3.788210 -2.698702
H -2.629847 0.534098 5.434301
H -1.401988 -0.687118 5.872160
H -0.892688 0.930816 5.313305
H 1.064126 -2.091642 2.453544
H 3.775339 -3.256577 -1.545579
H 2.780400 -3.848298 2.592155
H 4.145589 -4.445548 0.601816
H 0.916717 1.084250 -5.310983
H 1.420564 -0.523326 -5.901611
H 2.651848 0.679462 -5.423898
H -1.751927 4.735786 -0.919980
H -1.622627 4.122607 -2.584490
H -3.021340 5.104269 -2.104392
H -4.387190 1.572906 -2.276852
H -4.593549 3.215998 -2.915657
H -3.175063 2.257269 -3.384012
H -4.783288 4.113952 -0.500459
H -4.583036 2.459565 0.110515
H -3.499870 3.753886 0.671409
H 2.344307 4.584707 0.209105
H 1.599821 4.514301 1.822986
H 3.250847 5.136389 1.631558
H 3.737642 1.683363 3.113106
H 4.087432 3.405860 3.359906
H 2.426059 2.806411 3.538017
H 5.160788 3.507694 1.011856
H 4.803908 1.782834 0.792292
H 4.229958 2.970327 -0.400554
H -3.108399 -1.819092 3.783842
H 3.104716 -1.715246 -3.809110

C4 – State T₁

C -3.351222 -3.672094 -0.812587
C -3.232339 -3.088611 0.407541
C -2.240091 -2.042476 0.585521
C -1.348254 -1.612828 -0.565350
C -1.538359 -2.252660 -1.766185
C -2.512619 -3.270299 -1.931144
H -4.085796 -4.456686 -0.969379
H -3.855661 -3.383266 1.244715
H -0.935165 -1.981045 -2.627991
H -2.642665 -3.756575 -2.891344

C -2.010173 -1.350774 1.764919
N -1.012197 -0.375816 1.755765
N -2.565797 -1.393228 3.016067
N -0.939460 0.171817 2.929830
N -1.865892 -0.446046 3.654460
C -2.096539 -0.109102 5.051481
H -3.130071 0.218751 5.173005
H -1.912014 -0.990680 5.667414
H -1.409806 0.691414 5.318042
C 1.384094 -1.634732 0.418403
C 2.243469 -1.973279 -0.658918
C 1.569542 -2.337530 1.613782
C 3.228437 -2.964209 -0.557765
C 2.548895 -3.330938 1.725772
H 0.950465 -2.116080 2.478078
C 3.377993 -3.648822 0.644569
H 3.864175 -3.189710 -1.408818
H 2.667220 -3.861587 2.666627
H 4.134612 -4.420760 0.742131
C 2.006670 -1.188896 -1.854295
N 1.013922 -0.254266 -1.794361
N 2.572234 -1.161283 -3.057635
N 0.943721 0.367881 -2.949242
N 1.884203 -0.196987 -3.676485
C 2.149016 0.201186 -5.054848
H 1.467618 1.013076 -5.298893
H 1.977322 -0.652902 -5.710443
H 3.184386 0.533157 -5.133514
Ir -0.011353 -0.122387 -0.014394
C -1.341045 1.310793 -0.627995
C 1.304917 1.270839 0.708732
N -2.093830 2.114327 -1.008366
N 2.065044 2.039837 1.142277
C -3.026784 3.115918 -1.497259
C -2.208399 4.350933 -1.911759
C -3.772257 2.510550 -2.699192
C -3.996532 3.447622 -0.349934
H -1.657127 4.756909 -1.059693
H -1.499847 4.099843 -2.705214
H -2.889241 5.120472 -2.284304
H -4.326239 1.616020 -2.403195
H -4.481600 3.247076 -3.085335
H -3.074267 2.247451 -3.498083
H -4.707979 4.202815 -0.693577
H -4.553871 2.559210 -0.041837
H -3.457347 3.844930 0.513886
C 3.013779 2.990857 1.697019
C 2.459372 4.404112 1.447707
C 3.139133 2.697650 3.202200
C 4.356104 2.782832 0.974605
H 2.344144 4.594337 0.377556
H 1.490872 4.535134 1.937116
H 3.158131 5.137721 1.857876
H 3.503486 1.681228 3.371990
H 3.850498 3.400517 3.643280
H 2.175638 2.816307 3.704546
H 5.088432 3.488277 1.375408
H 4.728941 1.767362 1.130750
H 4.252468 2.961196 -0.098788

A1 – State ³MC

C 0.649843 -3.531095 1.690571

C 0.247747 -2.497328 0.834098
C -0.527761 -1.410947 1.331864
C -0.872360 -1.402805 2.695542
C -0.464463 -2.435373 3.539391
C 0.296319 -3.498592 3.038310
C 0.578053 -2.451721 -0.592095
C 1.349034 -3.390428 -1.287417
Ir -1.059865 -0.053581 -0.097088
N 0.065310 -1.371772 -1.252805
N -2.282024 1.133521 1.103588
C -1.822303 1.952128 2.071628
C -3.622558 1.048830 0.855269
C -3.977210 0.129558 -0.228345
C -2.888940 -0.516511 -0.882020
C -3.172341 -1.410514 -1.930108
C -4.488277 -1.657390 -2.319929
C -5.549704 -1.016585 -1.669519
C -5.296142 -0.128092 -0.626155
C 0.060549 1.514137 -0.636726
N 0.725604 2.428537 -0.946046
C 1.606318 3.532188 -1.280970
C 2.625057 3.015323 -2.312195
C 0.741649 4.663169 -1.865378
C 2.308309 3.976831 0.015321
C 3.893457 0.329523 0.344487
N 5.045182 0.158700 0.493290
C 6.467422 -0.058915 0.680517
C 7.201615 1.224401 0.253488
C 6.707336 -0.362808 2.169817
C 6.882386 -1.251264 -0.199326
H -6.572985 -1.211029 -1.974383
H -6.130463 0.356584 -0.129357
H -2.365542 -1.921653 -2.444861
H -4.690311 -2.350708 -3.131233
H -1.463500 -0.590254 3.105049
H 1.236978 -4.364218 1.317653
H -0.739008 -2.414511 4.590062
H 0.611797 -4.301251 3.697121
H 3.208319 2.190956 -1.894465
H 2.120936 2.672479 -3.219554
H 3.305223 3.828733 -2.578060
H -0.000080 5.002455 -1.137639
H 1.386531 5.507218 -2.123376
H 0.224807 4.330894 -2.769409
H 2.981240 4.807707 -0.212399
H 1.579338 4.312747 0.757441
H 2.892983 3.154861 0.435818
H 7.010445 1.449583 -0.799090
H 6.879694 2.075906 0.858827
H 8.277682 1.087473 0.389971
H 6.161324 -1.258910 2.476391
H 7.774579 -0.532106 2.336369
H 6.386242 0.474916 2.794473
H 7.952752 -1.436251 -0.075463
H 6.337565 -2.154233 0.088659
H 6.685069 -1.043037 -1.254219
C 1.593562 -3.221583 -2.644534
C 0.305156 -1.206414 -2.569477
C 1.063733 -2.107975 -3.300299
H 1.754944 -4.246291 -0.762987
H 2.191081 -3.947875 -3.184882
H 1.230410 -1.935573 -4.356660
H -0.132026 -0.327354 -3.026661

C -4.518984 1.811409 1.612753
C -4.045485 2.653507 2.611165
C -2.670695 2.728491 2.846234
H -5.581658 1.743443 1.416508
H -4.739122 3.245394 3.198572
H -2.257484 3.372048 3.613351
H -0.748602 1.965750 2.212220

N2 – State ³MC

C 0.353271 -1.729625 -3.736789
C 0.619160 -2.664365 -2.751655
N 0.176849 -2.154178 -1.573346
N -0.364654 -0.920097 -1.772444
C -0.261607 -0.652354 -3.079809
C 0.182550 -2.628203 -0.240444
C -0.355318 -1.730319 0.713796
C -0.368342 -2.155639 2.054075
C 0.129286 -3.407959 2.414637
C 0.651199 -4.267960 1.441939
C 0.680194 -3.883322 0.100417
Ir -1.069094 0.017997 -0.085190
C 0.032610 1.657743 -0.423256
N 0.691742 2.603954 -0.626723
C 1.574425 3.733618 -0.855345
C 2.421518 3.925286 0.415875
H 0.574954 -1.814772 -4.788724
C -3.071876 -0.125836 -0.510463
C -3.920034 0.321030 0.531796
C -5.309251 0.279393 0.444537
C -5.887006 -0.221638 -0.723281
C -5.082335 -0.672482 -1.775593
C -3.692190 -0.625655 -1.668971
N -3.249283 0.817282 1.674781
N -1.887515 0.785828 1.638006
C -1.451702 1.305105 2.792051
C -2.546656 1.675443 3.588449
C -3.671159 1.352948 2.849261
H -2.521399 2.119097 4.571045
C 2.461245 3.389015 -2.065016
C 0.697182 4.966588 -1.135094
C 3.833449 0.211721 0.070692
N 4.941169 -0.076564 0.330658
C 6.309783 -0.437796 0.649707
C 6.849142 -1.306823 -0.500035
C 7.121891 0.862229 0.786612
C 6.296065 -1.221681 1.973949
H -6.968076 -0.259799 -0.807333
H -5.937049 0.625119 1.258694
H -3.082948 -0.981911 -2.493173
H -5.542290 -1.061304 -2.678896
H -0.773556 -1.503955 2.821095
H 1.082425 -4.554322 -0.650962
H 0.110213 -3.717530 3.455083
H 1.036051 -5.242387 1.724131
H 3.055503 2.494404 -1.862524
H 1.853761 3.220028 -2.958016
H 3.138824 4.224718 -2.258639
H 0.047686 5.184183 -0.283268
H 1.343814 5.830675 -1.308644
H 0.078034 4.811293 -2.022405
H 3.099257 4.770068 0.267156
H 1.785630 4.137618 1.279339

H 3.014098 3.030090 0.620179
H 7.107320 1.429737 -0.147654
H 6.718675 1.490214 1.585477
H 8.159387 0.615951 1.027789
H 5.698440 -2.132291 1.880200
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H 5.883434 -0.612554 2.782540
H 7.881404 -1.593812 -0.282438
H 6.251980 -2.215549 -0.612868
H 6.832925 -0.756062 -1.444257
H -4.720237 1.465771 3.071676
H 1.083452 -3.636091 -2.805147
H -0.392844 1.382394 2.986223
H -0.629039 0.283425 -3.472396

N3 – State ³MC

C 0.808775 -1.627796 -3.416364
C 1.143732 -2.545715 -2.438100
N 0.556038 -2.079862 -1.311419
N -0.101460 -0.933696 -1.608506
N 0.043892 -0.648425 -2.874890
C 0.487774 -2.509921 0.038905
C -0.252597 -1.655794 0.889598
C -0.346924 -2.027615 2.241252
C 0.267622 -3.191903 2.704639
C 0.988783 -4.012003 1.830016
C 1.105761 -3.675267 0.479931
Ir -1.077790 -0.033785 -0.053835
C -0.073785 1.698032 -0.254503
N 0.521047 2.697693 -0.363615
C 1.305252 3.915276 -0.478986
C 1.805538 4.278683 0.930579
H 1.074711 -1.622248 -4.461502
C -2.983709 -0.281019 -0.774587
C -4.001273 0.089885 0.135543
C -5.357988 -0.019844 -0.150479
C -5.728387 -0.521119 -1.399928
C -4.752515 -0.898014 -2.328990
C -3.396173 -0.780143 -2.021479
N -3.528095 0.593533 1.374730
N -2.183226 0.643914 1.527924
N -1.883907 1.128084 2.703695
C -3.054737 1.397356 3.331378
C -4.109947 1.063728 2.502443
H -3.078265 1.809292 4.327783
C 2.478738 3.618889 -1.429357
C 0.385362 5.011338 -1.045140
C 3.732750 0.137229 -0.012495
N 4.877854 -0.058617 0.155513
C 6.292733 -0.302663 0.365074
C 6.757666 -1.324060 -0.687793
C 7.032601 1.036408 0.198528
C 6.470454 -0.858206 1.789076
H -6.780910 -0.615052 -1.644775
H -6.113616 0.274641 0.569676
H -2.654347 -1.071241 -2.757451
H -5.052531 -1.284026 -3.298211
H -0.896470 -1.400187 2.934826
H 1.665972 -4.310460 -0.197471
H 0.186131 -3.462620 3.752703
H 1.463256 -4.916424 2.195413
H 3.089267 2.797522 -1.045778

H 2.114793 3.354354 -2.425546
H 3.101191 4.513601 -1.512024
H -0.458163 5.196805 -0.375319
H 0.959380 5.935869 -1.146952
H 0.002419 4.728893 -2.029000
H 2.396694 5.195981 0.869472
H 0.966756 4.449188 1.610223
H 2.435964 3.483686 1.336519
H 6.880065 1.442472 -0.804969
H 6.681294 1.768191 0.930783
H 8.103742 0.878908 0.350676
H 5.923421 -1.796864 1.910904
H 7.531456 -1.047002 1.973356
H 6.110102 -0.142825 2.533011
H 7.823899 -1.523452 -0.551005
H 6.211628 -2.265391 -0.583714
H 6.603108 -0.937913 -1.698804
H -5.177903 1.124792 2.629223
H 1.728773 -3.449846 -2.463336

N4 – State ³MC

N 1.222931 -1.708974 -3.113845
C 1.341279 -2.595373 -2.133057
N 0.632768 -2.170186 -1.073067
N 0.084508 -0.990094 -1.436320
N 0.440234 -0.719220 -2.658235
C 0.363592 -2.614393 0.247270
C -0.427985 -1.722517 1.007738
C -0.722734 -2.103418 2.327405
C -0.248201 -3.311299 2.841051
C 0.527757 -4.167606 2.051897
C 0.843337 -3.824124 0.735981
Ir -1.027290 -0.044972 -0.011751
C 0.111434 1.623313 -0.061889
N 0.780152 2.578102 -0.103758
C 1.654249 3.738278 -0.163958
C 2.464038 3.774201 1.144625
C -2.829088 -0.108773 -0.995735
C -3.930645 0.331918 -0.226227
C -5.240095 0.347201 -0.692611
C -5.472730 -0.097211 -1.995422
C -4.411351 -0.539868 -2.792849
C -3.105097 -0.548315 -2.301199
N -3.588576 0.769446 1.080691
N -2.281666 0.689573 1.423200
N -2.138926 1.132907 2.638559
N -3.337854 1.506340 3.111322
C -4.224675 1.281081 2.149368
C 2.571648 3.556893 -1.385837
C 0.763897 4.985036 -0.305919
C 3.359569 -0.357236 -0.382936
N 4.501922 -0.299582 -0.118913
C 5.916883 -0.252830 0.201136
C 6.691600 -0.039653 -1.111216
C 6.145421 0.917814 1.173235
C 6.296290 -1.593683 0.854480
H -6.484826 -0.096501 -2.384931
H -6.059748 0.691323 -0.071309
H -2.297869 -0.892292 -2.938597
H -4.605384 -0.880496 -3.804907
H -1.318860 -1.453372 2.958500
H 1.444107 -4.486136 0.122123

H -0.483900 -3.588662 3.863545
H 0.889918 -5.105722 2.458070
H 3.160884 2.641076 -1.294760
H 1.987772 3.512664 -2.308708
H 3.252868 4.409436 -1.444693
H 0.093581 5.085484 0.551374
H 1.403275 5.870145 -0.353185
H 0.167527 4.936770 -1.220392
H 3.131615 4.639310 1.120312
H 1.803671 3.867537 2.010412
H 3.067732 2.869816 1.253427
H 5.851011 1.866097 0.715706
H 5.571271 0.777146 2.092869
H 7.206524 0.971534 1.431079
H 6.107086 -2.426266 0.171721
H 7.360406 -1.584898 1.105219
H 5.724165 -1.754411 1.772072
H 7.762741 -0.001737 -0.895674
H 6.505909 -0.859610 -1.809896
H 6.399004 0.900124 -1.586816
H -5.284402 1.472167 2.199551
H 1.906450 -3.512497 -2.166694

C2 – State ³MC

C 3.661503 2.625643 -1.546852
C 3.255311 1.465453 -0.931541
N 1.873813 1.516784 -0.801820
C 1.461167 2.668637 -1.315718
N 2.520705 3.367967 -1.780099
C 3.885293 0.267308 -0.400071
C 2.984223 -0.665987 0.195026
C 3.522040 -1.847274 0.735818
C 4.894888 -2.097487 0.690089
C 5.763195 -1.170821 0.101064
C 5.259823 0.010121 -0.444933
Ir 0.992827 -0.118037 0.112704
C 0.052212 1.008798 1.460544
N -0.505557 1.677075 2.248793
C -1.250622 2.502344 3.178949
C -0.437619 2.601198 4.482519
C 2.469277 4.683312 -2.415322
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C -0.439832 -2.693265 -0.044621
C -0.895111 -3.800861 0.630215
N -0.510634 -3.645291 1.947274
C 0.156707 -2.474646 2.055400
C -0.784389 -4.581607 3.035713
C -0.487242 -2.184324 -1.405793
C 0.131691 -0.911290 -1.588131
C 0.119745 -0.352595 -2.878316
C -0.478266 -1.024730 -3.945995
C -1.079716 -2.273259 -3.748106
C -1.083440 -2.854006 -2.479780
C -1.431669 3.888061 2.533575
C -2.610070 1.821371 3.421286
C -3.743096 0.856643 -0.233472
N -4.847310 0.663898 -0.581907
C -6.210937 0.426797 -1.017249
C -6.186231 0.182894 -2.536449
C -6.737576 -0.809705 -0.267854
C -7.041361 1.675668 -0.672464
H 6.830073 -1.369148 0.066802

H 5.935711 0.727042 -0.903030
H 2.866789 -2.581895 1.193244
H 5.290702 -3.016708 1.112804
H 3.031488 5.405846 -1.820772
H 2.894222 4.626564 -3.419063
H 1.429577 5.001551 -2.482130
H 0.582782 0.612856 -3.055329
H -1.549277 -3.823971 -2.328460
H -0.475765 -0.576388 -4.935572
H -1.543439 -2.792982 -4.580933
H -0.327485 -4.202757 3.949177
H -0.359869 -5.558763 2.798623
H -1.861930 -4.676987 3.182455
H -3.157102 1.705661 2.482055
H -2.474161 0.835469 3.873851
H -3.202214 2.438044 4.102727
H 0.538050 3.058870 4.299444
H -0.983808 3.221110 5.198474
H -0.287031 1.612148 4.922988
H -1.987605 4.532142 3.219950
H -0.462906 4.351756 2.329676
H -1.990972 3.810576 1.597780
H -7.035341 1.860996 0.404931
H -6.646773 2.558120 -1.183031
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H -7.204925 0.002209 -2.890064
H -5.784632 1.052649 -3.063136
H -7.766290 -1.010225 -0.579122
H -6.128123 -1.688966 -0.492823
H -6.727584 -0.642622 0.812520
H 4.637127 2.984068 -1.833347
H -1.447357 -4.666239 0.301037
H 0.441341 3.015402 -1.365056
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C3 – State ³MC

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C 0.205301 -0.932564 -1.646720
C 0.197277 -0.378165 -2.937284
C -0.358182 -1.078891 -4.010558
C -0.917916 -2.346870 -3.818465
C -0.927126 -2.922092 -2.546835
Ir 1.011891 -0.109805 0.067628
C -0.015219 1.012325 1.369755
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C -1.395214 2.477248 3.050497
C -1.595129 3.857794 2.400391
C -0.569960 -4.393827 3.081911
C 3.012089 -0.568882 0.315929
C 3.913769 0.378862 -0.252699
C 5.296674 0.189353 -0.189986
C 5.808249 -0.943869 0.444520
C 4.939844 -1.881461 1.014152
C 3.556529 -1.696995 0.951330
C 3.264449 1.521301 -0.875017
N 1.895312 1.510521 -0.840319

N 1.385207 2.575479 -1.412119
N 2.433814 3.289666 -1.826789
C 3.613825 2.689103 -1.523163
C 2.219885 4.560462 -2.516691
C -2.741584 1.763895 3.269566
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C -3.753590 0.649477 -0.370647
N -4.898144 0.506988 -0.589310
C -6.311858 0.333618 -0.865901
C -6.736590 -1.039599 -0.316367
C -7.073504 1.469804 -0.160843
C -6.506849 0.401506 -2.390803
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H 5.971442 0.918234 -0.629601
H 2.901816 -2.434266 1.404540
H 5.343575 -2.759706 1.509670
H 2.685454 5.367082 -1.948743
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H 1.145797 4.721640 -2.582342
H 0.620887 0.605978 -3.108882
H -1.362685 -3.905731 -2.396512
H -0.355622 -0.634708 -5.001800
H -1.346989 -2.885891 -4.657160
H -0.038083 -3.926442 3.908161
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H -1.635829 -4.451612 3.308048
H -3.270424 1.635610 2.321746
H -2.590265 0.781650 3.724866
H -3.358821 2.367205 3.940445
H 0.363861 3.071412 4.198239
H -1.175381 3.198143 5.073099
H -0.438307 1.605393 4.807476
H -2.177591 4.488538 3.076899
H -0.633610 4.343106 2.213798
H -2.135720 3.767885 1.454894
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H -7.567160 0.274930 -2.625672
H -6.177162 1.367488 -2.782352
H -7.800668 -1.194553 -0.514271
H -6.172701 -1.842326 -0.798892
H -6.572081 -1.094376 0.763041
H 4.566028 3.123492 -1.780759
H -1.259459 -4.721351 0.337491

C4 – State ³MC

C 5.780618 -1.040931 0.509529
C 5.295342 0.050527 -0.211558
C 3.916857 0.259862 -0.280390
C 2.989370 -0.610853 0.361471
C 3.509458 -1.697949 1.081213
C 4.889399 -1.907658 1.152353
H 6.849790 -1.215046 0.571478
H 5.976608 0.731145 -0.712649
H 2.844136 -2.384905 1.593570
H 5.273572 -2.753897 1.714282
C 3.286085 1.358023 -0.985760
N 1.923108 1.394752 -0.955550
N 3.748859 2.390696 -1.680382
N 1.513014 2.448565 -1.625977

N 2.625363 3.016706 -2.043199
C 2.625557 4.239168 -2.840518
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H 3.112009 4.037760 -3.795090
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C 0.103759 -0.569986 -2.887431
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C -0.499841 -1.328765 -3.893866
H 0.554205 0.383081 -3.143488
C -1.098414 -2.560040 -3.602846
H -1.562908 -3.995576 -2.054966
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H -1.563063 -3.140044 -4.393414
C -0.439842 -2.665086 0.107665
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N -0.502564 -3.415360 2.041352
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H -0.338562 -5.260770 2.998396
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Ir 0.995482 -0.116535 0.080113
C 0.025210 1.141098 1.306579
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H -3.189992 1.991865 2.191196
H -2.565347 1.205765 3.657719
H -3.249250 2.841038 3.752978
H 0.507355 3.356689 3.998030
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H -1.947569 4.832643 2.769323
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H -6.036307 1.457642 -2.761507
H -7.852960 -1.080730 -0.616038
H -6.252562 -1.803905 -0.875336
H -6.657936 -1.080161 0.696413