

Supplementary information

Thermally Induced Inter-Ring Haptotropic Rearrangements in π -Complexes of Molybdenum with Nitrogen Containing Polyaromatic Heterocycles: a DFT Study

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Table of Cartesian coordinates of all the computed stationary points

I-a

C	-0.73115	1.55072	2.60015
C	-1.25516	0.34216	3.03618
C	-0.41820	-0.78018	3.28314
C	0.95542	-0.71825	3.09177
C	1.53181	0.51724	2.68204
C	0.67727	1.65917	2.45101
H	-2.33232	0.24331	3.18108
H	-0.87122	-1.71376	3.62234
H	1.58851	-1.58243	3.30088
N	1.41731	2.79009	2.11546
C	2.87038	0.98342	2.45436
H	3.78915	0.43232	2.63623
H	-1.36571	2.41730	2.41123
Mo	1.81775	1.33159	0.35786
P	1.35496	3.23633	-1.02403
P	1.18150	-0.74534	-0.74698
P	3.96629	1.11352	-0.72044
H	0.32895	1.39309	-0.54334
C	1.81782	-2.38514	-0.08706
C	-0.64751	-1.11341	-0.63470
C	1.41506	-1.04981	-2.58358
C	2.54165	4.69178	-1.02792
C	0.98841	3.09114	-2.85150
C	-0.18339	4.15575	-0.49522
H	-0.87843	-2.12455	-1.00279
H	-0.96245	-1.01990	0.41385
H	-1.19547	-0.36754	-1.22544
H	1.39227	-3.22853	-0.65204

H 2.91223 -2.42666 -0.13822
H 1.51759 -2.46992 0.96588
H 0.93475 -1.99026 -2.89484
H 0.97057 -0.21216 -3.13781
H 2.48483 -1.09911 -2.82812
H -0.33319 5.06414 -1.09766
H -1.05011 3.49013 -0.60454
H -0.07302 4.41897 0.56480
H 2.13026 5.54232 -1.59257
H 2.70521 4.99747 0.01500
H 3.50830 4.40625 -1.46349
H 0.74251 4.07409 -3.28177
H 1.84415 2.66312 -3.38729
H 0.12949 2.41666 -2.97235
C 4.87994 -0.53348 -0.71736
C 4.28565 1.54462 -2.52177
C 5.35457 2.13372 0.03252
H 5.33282 1.33776 -2.79060
H 3.62377 0.95370 -3.16819
H 4.08052 2.60859 -2.69709
H 6.29615 1.98679 -0.51769
H 5.08503 3.19792 0.01346
H 5.50691 1.83430 1.07857
H 5.91262 -0.41493 -1.07954
H 4.89546 -0.93293 0.30598
H 4.36319 -1.25579 -1.36327
C 2.74714 2.38565 2.16754
H 3.54148 3.12268 2.08942

I-b

C -1.23083 1.16069 2.28477
C -1.39016 -0.18143 2.73098
C -0.26029 -1.01071 2.96217
C 1.06091 -0.53039 2.72249
C 1.24970 0.87845 2.50857
C 0.08524 1.73791 2.31652
H -2.39180 -0.58793 2.87841
H -0.41231 -2.05476 3.23926
H 1.91051 -1.19268 2.89794
N 0.43849 3.04217 2.17746
C 2.35954 1.77227 2.50771
H 3.40760 1.52710 2.65781
H -2.10435 1.79286 2.12592
Mo -0.14002 -0.24855 0.75440
P -2.02779 -1.31418 -0.30367
P 1.83971 -1.02532 -0.48131
P -0.31472 1.58319 -0.95848
H -0.09644 -1.95051 0.55716
C 3.49414 -0.23908 -0.09312

C 2.29760 -2.80719 -0.14492
C 1.98758 -1.08388 -2.35405
C -3.61603 -0.35218 -0.58014
C -1.87476 -2.17114 -1.96266
C -2.75480 -2.75390 0.64854
H 3.26171 -3.06678 -0.60758
H 2.35533 -2.96206 0.94064
H 1.51123 -3.46311 -0.54175
H 4.28629 -0.67360 -0.72097
H 3.45044 0.84616 -0.24576
H 3.73309 -0.41610 0.96347
H 2.92061 -1.58539 -2.65301
H 1.13321 -1.63473 -2.76993
H 1.98695 -0.06900 -2.77303
H -3.61326 -3.18591 0.11325
H -1.98072 -3.52138 0.78065
H -3.08438 -2.42125 1.64161
H -4.41196 -0.99955 -0.97845
H -3.94012 0.07163 0.38067
H -3.44896 0.47880 -1.27757
H -2.82092 -2.65248 -2.25468
H -1.57937 -1.45219 -2.73656
H -1.08964 -2.93587 -1.88173
C 1.23679 2.57371 -1.26029
C -0.83355 1.28667 -2.73371
C -1.47315 2.98234 -0.53855
H -0.77073 2.22880 -3.29890
H -0.18427 0.53984 -3.20653
H -1.86897 0.92419 -2.77433
H -1.47374 3.72958 -1.34641
H -2.49174 2.59838 -0.39423
H -1.11702 3.44425 0.39440
H 1.01517 3.46555 -1.86511
H 1.64229 2.88182 -0.28696
H 1.98426 1.96311 -1.78333
C 1.80260 3.04401 2.32892
H 2.34578 3.98976 2.29400

I-TS

C -1.77412 0.42348 3.38376
C -1.66533 -0.96819 3.33742
C -0.44218 -1.59350 2.97596
C 0.74636 -0.86487 2.74761
C 0.63122 0.56140 2.73783
C -0.64534 1.20841 3.05921
H -2.52930 -1.59189 3.57048
H -0.39416 -2.68435 2.95890
H 1.70962 -1.37374 2.70480
N -0.53235 2.57353 3.01623

C 1.50380 1.64191 2.39201
H 2.56703 1.58672 2.17542
H -2.70516 0.91246 3.67801
Mo 0.10304 -0.06026 0.55342
P -1.78853 -0.96588 -0.61104
P 2.06088 -0.86817 -0.50631
P 0.09395 1.79216 -0.99974
H 0.10564 -1.66271 -0.00812
C 3.67830 -0.08498 0.03725
C 2.51307 -2.66135 -0.19924
C 2.32232 -0.85964 -2.36440
C -3.32585 0.09779 -0.77429
C -1.65738 -1.65925 -2.34399
C -2.58624 -2.46096 0.19327
H 3.51224 -2.89770 -0.59426
H 2.48996 -2.86437 0.87999
H 1.76829 -3.30735 -0.68426
H 4.52580 -0.52412 -0.51049
H 3.65403 0.99832 -0.13240
H 3.81799 -0.26445 1.11221
H 3.26953 -1.35249 -2.63167
H 1.48940 -1.38932 -2.84601
H 2.34138 0.17248 -2.73806
H -3.45615 -2.80763 -0.38451
H -1.84390 -3.26754 0.26229
H -2.90342 -2.19456 1.20939
H -4.17086 -0.49454 -1.15632
H -3.58197 0.49966 0.21599
H -3.14333 0.94055 -1.45321
H -2.63062 -2.04240 -2.68701
H -1.29768 -0.89458 -3.04214
H -0.93261 -2.48541 -2.32751
C 1.64884 2.83182 -1.18116
C -0.38066 1.73589 -2.81525
C -1.07745 3.14381 -0.44023
H -0.29164 2.73899 -3.25933
H 0.27105 1.04238 -3.36237
H -1.41911 1.39668 -2.92283
H -0.94738 4.05266 -1.04758
H -2.11305 2.79096 -0.53293
H -0.89426 3.37141 0.61936
H 1.44384 3.74631 -1.75767
H 2.00877 3.10229 -0.18028
H 2.43326 2.25988 -1.69538
C 0.74290 2.81605 2.63689
H 1.09272 3.84319 2.52049

II-a

Mo 0.29014 0.42870 -0.18378

C -1.66182 0.31124 1.23578
N -1.36252 1.62906 0.85037
C -0.14932 2.13280 1.23977
C 0.88353 1.32839 1.82809
C 0.65821 -0.05359 2.04426
C -0.66801 -0.57413 1.81477
C -1.06538 -1.90489 2.15156
C -2.36672 -2.33783 1.96638
C -3.34206 -1.46042 1.42960
C -2.99032 -0.17056 1.06922
H 0.00885 3.19427 1.04692
H 1.83232 1.78915 2.10613
H 1.42176 -0.68058 2.50506
H -0.32697 -2.56661 2.61178
H -2.64667 -3.35436 2.24930
H -4.37148 -1.79982 1.30510
H -3.73402 0.53167 0.68944
P 2.18964 1.62710 -1.07267
P -0.97610 0.76155 -2.27388
P 1.24157 -1.69683 -0.95149
C 3.87701 1.09121 -0.43622
C 2.64314 1.79192 -2.89085
C 2.32416 3.45141 -0.64341
C -0.05431 -2.98693 -1.35574
C 2.34351 -1.94243 -2.45627
C 2.27178 -2.67619 0.27178
C -2.72972 0.10412 -2.34578
C -1.34298 2.56057 -2.62864
C -0.44916 0.19442 -3.98546
H -1.15718 0.55358 -4.74802
H 0.55557 0.56142 -4.22597
H -0.43375 -0.90444 -4.01438
H -2.03159 2.67363 -3.48042
H -1.79375 2.98861 -1.72275
H -0.40948 3.09891 -2.84118
H -3.19437 0.32707 -3.31843
H -2.73046 -0.98133 -2.17837
H -3.31504 0.57352 -1.54645
H 0.40752 -3.96386 -1.56645
H -0.74423 -3.07646 -0.50596
H -0.63073 -2.66404 -2.23358
H 2.56635 -3.00976 -2.60844
H 1.84275 -1.54930 -3.35062
H 3.29079 -1.40182 -2.32427
H 2.59700 -3.63794 -0.15348
H 3.15392 -2.08756 0.55874
H 1.67447 -2.86538 1.17310
H 4.68077 1.75050 -0.79919
H 3.86036 1.10527 0.66226

H 4.08610 0.06148 -0.75654
H 3.58509 2.34955 -3.00636
H 2.75656 0.79958 -3.34540
H 1.84793 2.33199 -3.42282
H 3.25065 3.88497 -1.04893
H 1.46017 3.98717 -1.05951
H 2.32079 3.58413 0.44669

II-b

Mo -1.20787 -1.58922 1.09792
C -2.15522 0.06199 2.62928
N -2.59835 1.34441 2.43317
C -1.76666 2.34649 2.68758
C -0.43370 2.17018 3.13632
C 0.04528 0.88620 3.31980
C -0.80387 -0.23562 3.07647
C -0.40014 -1.60709 3.26756
C -1.34657 -2.65449 3.10849
C -2.68707 -2.36948 2.68717
C -3.04909 -1.03932 2.35593
H -2.16139 3.35547 2.52923
H 0.19400 3.03990 3.33706
H 1.05693 0.71564 3.69631
H 0.60933 -1.82763 3.61743
H -1.05583 -3.67950 3.34407
H -3.41437 -3.17269 2.57534
H -4.06125 -0.79826 2.02957
P 0.92899 -0.91849 0.08662
P -2.48487 -0.82263 -0.85708
P -0.99796 -3.81857 0.19213
C 2.47029 -1.07386 1.14632
C 1.65461 -1.62881 -1.49624
C 1.05648 0.89681 -0.35750
C -2.26097 -5.09632 0.74056
C -1.01527 -4.25771 -1.63605
C 0.55485 -4.76581 0.67270
C -4.12765 -1.68688 -1.12521
C -3.08680 0.95023 -0.82019
C -1.88554 -0.82508 -2.64101
H -2.67589 -0.46459 -3.31729
H -1.01632 -0.15897 -2.73446
H -1.58371 -1.83411 -2.94788
H -3.75776 1.15718 -1.66807
H -3.59842 1.14773 0.13090
H -2.22003 1.62412 -0.87373
H -4.69388 -1.22792 -1.95042
H -3.95556 -2.74832 -1.35005
H -4.71743 -1.62507 -0.20099
H -2.03168 -6.08428 0.31377

H -2.26664 -5.17778 1.83557
H -3.26077 -4.78246 0.41121
H -0.84777 -5.33636 -1.77819
H -1.98991 -3.99301 -2.06847
H -0.23452 -3.70035 -2.16857
H 0.53029 -5.80541 0.31074
H 1.43913 -4.26262 0.25861
H 0.64690 -4.76150 1.76754
H 3.36185 -0.70183 0.61857
H 2.33420 -0.49801 2.07069
H 2.61982 -2.12844 1.41537
H 2.59352 -1.11725 -1.75830
H 1.86304 -2.69984 -1.36831
H 0.93955 -1.51095 -2.32057
H 2.07518 1.15790 -0.68332
H 0.34987 1.12693 -1.16664
H 0.78218 1.50033 0.51796

II-IM1

Mo 0.32334 -0.07942 -0.31943
C -1.87964 0.95837 1.65135
N -1.90958 2.29892 1.87226
C -0.73873 2.92025 2.10259
C 0.51080 2.29245 2.10443
C 0.59887 0.89657 1.86688
C -0.64589 0.17292 1.71576
C -0.69413 -1.26106 1.54687
C -1.92337 -1.85830 1.20907
C -3.11051 -1.09354 1.14440
C -3.09990 0.27327 1.39304
H -0.80186 3.99624 2.29436
H 1.40956 2.87646 2.31106
H 1.50721 0.34911 2.14138
H 0.14859 -1.88043 1.86659
H -1.97670 -2.93948 1.07525
H -4.05338 -1.59763 0.92283
H -4.01611 0.86510 1.38431
P 2.30032 1.09735 -0.93247
P -0.89867 0.72257 -2.17479
P 1.09877 -2.09136 -1.33091
C 3.72125 1.03126 0.30208
C 3.31284 0.75758 -2.48039
C 2.18065 2.96487 -1.11356
C 0.01939 -3.62169 -1.14738
C 1.47462 -2.30780 -3.16170
C 2.68656 -2.80083 -0.61501
C -2.41848 -0.30276 -2.57533
C -1.68876 2.39636 -1.87943
C -0.27443 1.01370 -3.92489

H -1.08761 1.36027 -4.58118
H 0.51550 1.77766 -3.90829
H 0.14780 0.08575 -4.33209
H -2.33094 2.67849 -2.72793
H -2.28531 2.36082 -0.95804
H -0.90664 3.15660 -1.75044
H -3.04956 0.20053 -3.32406
H -2.10360 -1.28025 -2.96542
H -2.99252 -0.45928 -1.65232
H 0.46144 -4.48200 -1.67271
H -0.08548 -3.86609 -0.08227
H -0.97980 -3.41992 -1.55553
H 1.91210 -3.29830 -3.36070
H 0.53300 -2.21944 -3.72194
H 2.16154 -1.52936 -3.51319
H 2.90285 -3.79776 -1.02922
H 3.52707 -2.12964 -0.83720
H 2.58553 -2.87627 0.47683
H 4.59910 1.57953 -0.07216
H 3.40379 1.47599 1.25456
H 4.00233 -0.01509 0.48602
H 4.13729 1.48167 -2.56641
H 3.73913 -0.25388 -2.43569
H 2.67587 0.83044 -3.37128
H 3.17668 3.42312 -1.21458
H 1.58512 3.20561 -2.00538
H 1.66742 3.38013 -0.23614

II-IM2

Mo 0.18846 0.58308 -0.60545
C -1.21533 -0.00738 1.61042
N -0.50429 1.13879 1.22426
C 0.78355 1.30050 1.72668
C 1.33093 0.38332 2.66722
C 0.61451 -0.71345 3.10504
C -0.68772 -0.95431 2.55866
C -1.47343 -2.08404 2.87374
C -2.72069 -2.29024 2.27995
C -3.23489 -1.35650 1.36428
C -2.49576 -0.21366 1.04686
H 1.19556 2.30646 1.65153
H 2.32416 0.59028 3.07224
H 1.02996 -1.40844 3.83630
H -1.08078 -2.81014 3.58992
H -3.30211 -3.17774 2.53593
H -4.21779 -1.51092 0.91656
H -2.89820 0.56357 0.39577
P 2.06436 1.83512 -1.30008
P -1.00778 0.79057 -2.67196

P 1.13157 -1.54437 -1.03760
C 3.72520 1.53920 -0.47245
C 2.65283 1.88301 -3.08250
C 1.92755 3.69201 -1.01600
C -0.08573 -2.97799 -1.06977
C 2.12846 -1.98413 -2.57047
C 2.33260 -2.21219 0.24304
C -2.71660 0.00491 -2.67049
C -1.50767 2.53412 -3.17779
C -0.43893 0.16366 -4.35057
H -1.12820 0.49119 -5.14391
H 0.57129 0.52724 -4.57628
H -0.41784 -0.93447 -4.32713
H -2.21419 2.53288 -4.02259
H -1.97043 3.03154 -2.31384
H -0.61097 3.10330 -3.46050
H -3.20358 0.12787 -3.65007
H -2.63171 -1.06370 -2.43404
H -3.33813 0.48287 -1.90200
H 0.43139 -3.95003 -1.08573
H -0.73044 -2.92435 -0.18124
H -0.72031 -2.89121 -1.96285
H 2.39806 -3.05167 -2.56862
H 1.55507 -1.75796 -3.47847
H 3.05101 -1.38675 -2.58230
H 2.64108 -3.24179 0.00462
H 3.21838 -1.56391 0.28066
H 1.85426 -2.19224 1.23093
H 4.46849 2.29293 -0.77499
H 3.59554 1.56764 0.61739
H 4.09070 0.54061 -0.74906
H 3.56335 2.49401 -3.17550
H 2.86401 0.86544 -3.43648
H 1.86851 2.31960 -3.71560
H 2.83931 4.21999 -1.33610
H 1.06505 4.07840 -1.57582
H 1.75563 3.88884 0.05150

II-TS1

Mo 0.33783 -0.03065 -0.32888
C -1.94547 0.79842 1.62792
N -2.11705 2.14948 1.69607
C -1.01243 2.90526 1.78890
C 0.29978 2.41246 1.84271
C 0.54091 1.01578 1.80316
C -0.62773 0.16282 1.70367
C -0.52924 -1.27798 1.65043
C -1.70584 -2.04375 1.54759
C -2.96817 -1.42307 1.48781

C -3.08904 -0.03569 1.53845
H -1.17850 3.98679 1.83476
H 1.12866 3.11041 1.97392
H 1.48188 0.60502 2.17936
H 0.41218 -1.76314 1.92599
H -1.64221 -3.13282 1.56198
H -3.86497 -2.04212 1.42340
H -4.06407 0.45331 1.51882
P 2.36312 1.07184 -0.89509
P -0.83207 0.84201 -2.18507
P 1.01855 -2.06560 -1.37710
C 3.73962 1.00231 0.38983
C 3.41584 0.65062 -2.39465
C 2.32174 2.93540 -1.15049
C -0.19800 -3.49883 -1.32335
C 1.49276 -2.26110 -3.18764
C 2.49257 -2.92274 -0.58669
C -2.37194 -0.15499 -2.58659
C -1.59219 2.52826 -1.89022
C -0.19739 1.11886 -3.93320
H -0.99708 1.49330 -4.59079
H 0.61716 1.85650 -3.91179
H 0.19717 0.17951 -4.34223
H -2.23449 2.81751 -2.73615
H -2.18599 2.50349 -0.96625
H -0.79496 3.27373 -1.76851
H -3.01420 0.38487 -3.29913
H -2.08048 -1.11944 -3.02416
H -2.93199 -0.34123 -1.65980
H 0.20119 -4.37361 -1.85905
H -0.39376 -3.76796 -0.27842
H -1.14965 -3.19701 -1.78100
H 1.85650 -3.28086 -3.38687
H 0.59923 -2.08152 -3.80203
H 2.26359 -1.53819 -3.47607
H 2.66380 -3.91634 -1.02886
H 3.39298 -2.30807 -0.72105
H 2.30909 -3.03369 0.49111
H 4.65291 1.49547 0.02403
H 3.41256 1.50289 1.31114
H 3.96652 -0.04657 0.62745
H 4.26779 1.34334 -2.46955
H 3.80411 -0.37301 -2.30597
H 2.81335 0.72232 -3.30949
H 3.33785 3.35172 -1.23123
H 1.76983 3.16125 -2.07371
H 1.79212 3.40695 -0.31307

II-TS2

Mo 0.30474 -0.08169 -0.32309
C -1.83757 0.99319 1.67656
N -1.83075 2.32428 1.94473
C -0.64517 2.90531 2.20675
C 0.58642 2.24558 2.18232
C 0.63423 0.85869 1.88844
C -0.62744 0.16967 1.72742
C -0.71406 -1.25830 1.52428
C -1.95236 -1.80364 1.13327
C -3.11719 -1.00223 1.07816
C -3.07438 0.35223 1.38038
H -0.68195 3.97352 2.44323
H 1.50166 2.79711 2.40502
H 1.53406 0.27930 2.12277
H 0.09986 -1.91246 1.84790
H -2.03572 -2.87742 0.96120
H -4.06947 -1.47159 0.82272
H -3.97395 0.96902 1.38398
P 2.27548 1.10690 -0.94097
P -0.91408 0.69250 -2.19574
P 1.10010 -2.09264 -1.31249
C 3.70369 1.04893 0.28474
C 3.28208 0.77969 -2.49544
C 2.13785 2.97426 -1.10896
C 0.03462 -3.63169 -1.12009
C 1.48173 -2.31807 -3.14067
C 2.69239 -2.78532 -0.58921
C -2.41001 -0.35591 -2.62268
C -1.73951 2.34911 -1.89804
C -0.27418 1.00673 -3.93613
H -1.08772 1.33423 -4.60166
H 0.49484 1.79127 -3.90681
H 0.17733 0.09157 -4.34104
H -2.36009 2.63786 -2.76039
H -2.36276 2.28533 -0.99621
H -0.97467 3.11925 -1.72976
H -3.03765 0.13824 -3.38040
H -2.07358 -1.32787 -3.00861
H -2.99432 -0.52263 -1.70817
H 0.49234 -4.49468 -1.62726
H -0.08111 -3.86347 -0.05314
H -0.96116 -3.44649 -1.54413
H 1.92292 -3.30833 -3.33252
H 0.54198 -2.23521 -3.70482
H 2.16813 -1.53997 -3.49418
H 2.92079 -3.78124 -0.99944
H 3.52700 -2.10610 -0.80943
H 2.58666 -2.85869 0.50243
H 4.58026 1.58920 -0.10355

H 3.39444 1.50884 1.23248
H 3.98242 0.00428 0.48091
H 4.09514 1.51574 -2.58791
H 3.72384 -0.22514 -2.44990
H 2.63941 0.84015 -3.38295
H 3.12839 3.44301 -1.21592
H 1.53103 3.21644 -1.99276
H 1.62972 3.37774 -0.22279

II-TS3

Mo 0.22271 0.47811 -0.53496
C -1.51049 -0.01501 1.52064
N -1.13470 1.21983 0.98788
C 0.09665 1.75667 1.35805
C 0.99679 1.02395 2.19773
C 0.62792 -0.19898 2.72184
C -0.67548 -0.73958 2.44494
C -1.14207 -1.95649 2.98487
C -2.38331 -2.47641 2.61397
C -3.18850 -1.78376 1.69059
C -2.76040 -0.56916 1.15301
H 0.21200 2.83292 1.22396
H 1.97157 1.45701 2.43071
H 1.31605 -0.76579 3.35249
H -0.50774 -2.49784 3.69152
H -2.72752 -3.42116 3.03785
H -4.15702 -2.19263 1.39747
H -3.39073 -0.00313 0.46657
P 2.12597 1.69513 -1.26552
P -0.93078 0.92318 -2.53098
P 1.19704 -1.60840 -1.15902
C 3.80215 1.25383 -0.52062
C 2.67760 1.81497 -3.05857
C 2.14638 3.53139 -0.86887
C -0.12179 -2.91354 -1.44658
C 2.30953 -1.98810 -2.62804
C 2.20686 -2.48113 0.16774
C -2.68807 0.23956 -2.56712
C -1.33713 2.72662 -2.86751
C -0.44321 0.39458 -4.27224
H -1.15475 0.77825 -5.02022
H 0.56546 0.74813 -4.51738
H -0.44435 -0.70409 -4.31304
H -2.05176 2.83450 -3.69832
H -1.76541 3.15843 -1.95257
H -0.41644 3.27402 -3.11256
H -3.18637 0.45760 -3.52454
H -2.66956 -0.84740 -2.40800
H -3.25722 0.70169 -1.74959

H 0.32931 -3.91502 -1.51916
H -0.83744 -2.89676 -0.61263
H -0.66203 -2.69243 -2.37694
H 2.53614 -3.06411 -2.68730
H 1.81531 -1.66722 -3.55471
H 3.25389 -1.43461 -2.52808
H 2.52820 -3.48259 -0.15835
H 3.09036 -1.87532 0.41078
H 1.59032 -2.57121 1.07215
H 4.58934 1.95846 -0.83186
H 3.72023 1.25697 0.57476
H 4.08469 0.23949 -0.83604
H 3.63415 2.35416 -3.13469
H 2.79312 0.81075 -3.48551
H 1.91957 2.35793 -3.63891
H 3.03857 4.01987 -1.28927
H 1.24330 4.00567 -1.27622
H 2.14737 3.67012 0.22079

II-TS4

Mo 0.04245 0.13146 -0.46964
C -0.85711 0.60139 1.57118
N -0.34084 1.86630 1.33644
C 0.47340 2.39038 2.27758
C 0.86817 1.70641 3.43072
C 0.51223 0.35349 3.56860
C -0.32476 -0.25409 2.62184
C -0.69378 -1.64418 2.61352
C -1.41889 -2.13551 1.55183
C -1.90759 -1.28207 0.49875
C -1.87850 0.13580 0.65597
H 0.83012 3.40790 2.09047
H 1.48133 2.20722 4.18031
H 0.88269 -0.23516 4.41171
H -0.34492 -2.29775 3.41537
H -1.63758 -3.20517 1.49541
H -2.59752 -1.71356 -0.22698
H -2.64033 0.80828 0.25983
P 1.95975 1.44448 -1.22103
P -1.21848 0.64611 -2.37751
P 0.87267 -1.96264 -1.29517
C 3.56960 1.05933 -0.32802
C 2.62342 1.56224 -2.97513
C 1.86339 3.27962 -0.87050
C -0.30438 -3.29598 -1.88012
C 2.13049 -2.10850 -2.68599
C 1.81985 -2.93100 0.01088
C -2.93351 -0.11076 -2.56786

C -1.70475 2.45246 -2.59914
C -0.63263 0.28747 -4.12617
H -1.33303 0.70329 -4.86709
H 0.36408 0.71148 -4.29535
H -0.57356 -0.80100 -4.26640
H -2.42258 2.59306 -3.42239
H -2.14189 2.81883 -1.65979
H -0.80148 3.04366 -2.80542
H -3.42413 0.26560 -3.47775
H -2.84735 -1.20387 -2.63468
H -3.56384 0.13558 -1.70280
H 0.23943 -4.21622 -2.14324
H -1.02734 -3.51131 -1.08398
H -0.85319 -2.93766 -2.76198
H 2.40885 -3.16023 -2.85459
H 1.71479 -1.69254 -3.61350
H 3.03587 -1.54393 -2.42412
H 2.16295 -3.90496 -0.37144
H 2.69082 -2.34176 0.33094
H 1.16914 -3.08108 0.88280
H 4.36332 1.77568 -0.59109
H 3.38718 1.09688 0.75540
H 3.90223 0.04371 -0.58503
H 3.57403 2.11675 -2.98645
H 2.78015 0.56584 -3.40529
H 1.89661 2.10285 -3.59686
H 2.74529 3.79614 -1.27840
H 0.95064 3.69446 -1.31609
H 1.81634 3.43621 0.21272

III-a

Mo -0.06188 0.38673 0.57027
C -2.00591 0.11419 2.03283
C -1.72756 1.46819 1.59038
N -0.59121 2.17343 1.91547
C 0.43159 1.42768 2.48808
C 0.32778 0.05339 2.83656
C -0.92292 -0.63029 2.63845
C -1.18082 -1.97389 3.05932
C -2.42592 -2.55038 2.88867
C -3.48360 -1.82070 2.28343
C -3.26998 -0.51997 1.86093
H 1.33139 1.98828 2.75123
H 1.15934 -0.44503 3.33586
H -0.38533 -2.52522 3.56579
H -2.60157 -3.57190 3.23178
H -4.46335 -2.28397 2.15820
H -4.08936 0.05539 1.42405

P 1.87074 1.57672 -0.27455
P -1.26085 0.79929 -1.52334
P 0.75632 -1.78647 -0.21742
C 3.52055 1.07689 0.47053
C 2.42028 1.67036 -2.06920
C 1.89757 3.41206 0.09019
C -0.58068 -3.03190 -0.61644
C 1.86171 -2.05199 -1.71475
C 1.76821 -2.79337 0.99869
C -3.06403 0.27533 -1.59355
C -1.48797 2.60732 -1.96723
C -0.77662 0.15397 -3.22314
H -1.44514 0.55530 -4.00034
H 0.25749 0.43393 -3.45928
H -0.84980 -0.94271 -3.23116
H -2.19591 2.73236 -2.80107
H -1.85500 3.14773 -1.08430
H -0.52059 3.04343 -2.25106
H -3.50393 0.50039 -2.57711
H -3.14436 -0.80126 -1.39205
H -3.62881 0.81092 -0.81964
H -0.15402 -4.02303 -0.83437
H -1.26419 -3.10259 0.24040
H -1.15486 -2.68569 -1.48681
H 2.04696 -3.12448 -1.88059
H 1.39550 -1.62348 -2.61076
H 2.82620 -1.55091 -1.55128
H 2.05092 -3.76948 0.57552
H 2.67627 -2.23370 1.26174
H 1.18085 -2.95106 1.91161
H 4.33750 1.73038 0.12768
H 3.44799 1.12408 1.56544
H 3.74812 0.03895 0.18997
H 3.35095 2.25156 -2.15775
H 2.58697 0.66238 -2.47007
H 1.64273 2.16066 -2.67042
H 2.87382 3.84945 -0.16768
H 1.11037 3.90181 -0.49793
H 1.67453 3.59104 1.14877
H -2.53587 2.05496 1.14542

III-b

Mo -0.29851 -0.14992 0.63240
C -1.10499 1.52154 2.18622
C -1.33681 2.91487 1.99804
N -0.46926 3.88381 2.26196
C 0.75081 3.49234 2.74284
C 1.12522 2.17904 2.93553
C 0.20794 1.11575 2.64804

C 0.49938 -0.27971 2.82395
C -0.52220 -1.24723 2.61503
C -1.83844 -0.85940 2.20447
C -2.08476 0.50031 1.87670
H 1.44537 4.30355 2.97983
H 2.10778 1.94680 3.35201
H 1.48345 -0.58601 3.17973
H -0.31098 -2.29632 2.82852
H -2.62195 -1.60539 2.07436
H -3.07854 0.80840 1.54458
P 1.82808 0.56911 -0.38329
P -1.59297 0.53105 -1.33402
P -0.04610 -2.38542 -0.25935
C 3.36718 0.42295 0.67628
C 2.56892 -0.12360 -1.96566
C 1.91295 2.38889 -0.80769
C -1.34949 -3.64587 0.23271
C 0.02440 -2.83895 -2.08274
C 1.48114 -3.32927 0.29854
C -3.17350 -0.43393 -1.63423
C -2.33125 2.25764 -1.32383
C -0.95597 0.57335 -3.10388
H -1.75877 0.85351 -3.80302
H -0.14941 1.31581 -3.18226
H -0.55450 -0.40606 -3.39166
H -2.89023 2.45511 -2.25122
H -3.01246 2.36040 -0.46928
H -1.53093 3.00135 -1.21339
H -3.76885 0.00812 -2.44816
H -2.93148 -1.47430 -1.89000
H -3.76650 -0.44002 -0.70949
H -1.10357 -4.64305 -0.16242
H -1.42539 -3.70757 1.32620
H -2.32401 -3.33004 -0.16342
H 0.19880 -3.91879 -2.20563
H -0.92778 -2.58060 -2.56576
H 0.82969 -2.28676 -2.58280
H 1.46689 -4.37456 -0.04677
H 2.37976 -2.83340 -0.09378
H 1.53499 -3.30617 1.39554
H 4.25190 0.81616 0.15258
H 3.21994 0.98522 1.60636
H 3.53342 -0.63305 0.92951
H 3.49460 0.41209 -2.22618
H 2.80692 -1.18782 -1.83010
H 1.85445 -0.02877 -2.79306
H 2.92392 2.67640 -1.13495
H 1.19690 2.61085 -1.61079
H 1.62924 2.97669 0.07527

H -2.32352 3.23307 1.64048

II-IM

Mo -0.19708 -0.01007 0.39841
C -1.66461 0.75735 1.98756
C -0.81105 1.90505 1.74897
N 0.12943 2.25147 2.75813
C 0.76505 1.21585 3.23020
C 0.48478 -0.12514 2.75359
C -0.91877 -0.38114 2.49506
C -1.62009 -1.62482 2.67071
C -2.98387 -1.68772 2.46183
C -3.73247 -0.53293 2.05983
C -3.08479 0.65725 1.80816
H 1.49849 1.38307 4.02992
H 1.09743 -0.94983 3.12445
H -1.06724 -2.50360 3.01017
H -3.50931 -2.63190 2.61982
H -4.81283 -0.61276 1.92900
H -3.64029 1.54048 1.48447
P 1.65692 1.45703 -0.12840
P -1.41417 0.49706 -1.61767
P 1.04394 -1.96111 -0.29657
C 3.28311 1.15676 0.75347
C 2.27802 1.49211 -1.89647
C 1.52195 3.30227 0.12110
C -0.17317 -3.34903 -0.65718
C 2.17397 -2.18590 -1.78277
C 2.13573 -2.82247 0.96839
C -2.94416 -0.59299 -1.73008
C -2.22092 2.18399 -1.80054
C -0.83462 0.29155 -3.39727
H -1.65446 0.48311 -4.10689
H -0.00768 0.97873 -3.61666
H -0.47338 -0.73709 -3.53583
H -2.88504 2.22466 -2.67748
H -2.79988 2.40758 -0.89468
H -1.43912 2.94940 -1.90630
H -3.57703 -0.29058 -2.57844
H -2.64205 -1.64031 -1.86656
H -3.51966 -0.51425 -0.79777
H 0.34415 -4.32057 -0.66266
H -0.96241 -3.36704 0.10751
H -0.63562 -3.18307 -1.63919
H 2.44337 -3.24507 -1.91396
H 1.67229 -1.82264 -2.68968
H 3.09667 -1.60671 -1.63681
H 2.57005 -3.75003 0.56492
H 2.94533 -2.14726 1.27736

H 1.53407 -3.06022 1.85590
H 4.05354 1.87268 0.42862
H 3.12331 1.25526 1.83455
H 3.62673 0.13395 0.54468
H 3.23855 2.02716 -1.94539
H 2.40171 0.48070 -2.29830
H 1.54802 2.02933 -2.51594
H 2.44054 3.80515 -0.21736
H 0.66772 3.67877 -0.45854
H 1.34390 3.51000 1.18457
H -1.24543 2.76645 1.23386

III-TS1

Mo -0.13536 -0.07752 0.48377
C -1.59350 0.76237 2.08633
C -0.45857 1.68531 1.93902
N 0.52928 1.70590 2.95717
C 0.86131 0.49707 3.35802
C 0.15951 -0.69430 2.96349
C -1.21266 -0.53368 2.58459
C -2.21175 -1.56033 2.61272
C -3.53411 -1.25099 2.32881
C -3.92385 0.05753 1.94512
C -2.95505 1.03951 1.78617
H 1.68392 0.41560 4.08022
H 0.49811 -1.66520 3.32793
H -1.93397 -2.56729 2.93164
H -4.29221 -2.03403 2.39991
H -4.96914 0.26887 1.71590
H -3.22487 2.04074 1.44276
P 1.52912 1.50505 -0.22841
P -1.40934 0.33794 -1.47588
P 1.28323 -1.87635 -0.32130
C 3.22158 1.30991 0.57182
C 2.09269 1.64838 -2.01709
C 1.32062 3.33899 0.08237
C 0.16055 -3.35177 -0.61296
C 2.34475 -2.00053 -1.86681
C 2.50713 -2.62638 0.88621
C -3.00498 -0.66251 -1.55729
C -2.12792 2.03966 -1.84443
C -0.82092 -0.07588 -3.21850
H -1.60738 0.13552 -3.95955
H 0.07864 0.49504 -3.47687
H -0.57712 -1.14699 -3.26378
H -2.81351 2.01849 -2.70565
H -2.66888 2.40077 -0.95941
H -1.30723 2.74004 -2.05507
H -3.58578 -0.43312 -2.46450

H -2.75543 -1.73345 -1.55293
H -3.61337 -0.45004 -0.66823
H 0.76233 -4.26596 -0.73074
H -0.52179 -3.47583 0.23894
H -0.43518 -3.19205 -1.52099
H 2.70338 -3.03129 -2.00900
H 1.76474 -1.69166 -2.74603
H 3.21590 -1.33772 -1.77026
H 3.00250 -3.50944 0.45419
H 3.26578 -1.87930 1.15511
H 1.97297 -2.91337 1.80065
H 3.91491 2.10255 0.25004
H 3.09308 1.35206 1.66117
H 3.64765 0.33276 0.30375
H 2.99835 2.27077 -2.08012
H 2.30033 0.66321 -2.44950
H 1.29785 2.12778 -2.60474
H 2.14681 3.89146 -0.38876
H 0.36809 3.68986 -0.33756
H 1.32964 3.52574 1.16398
H -0.71328 2.67609 1.55442

III-TS2

Mo -0.19453 -0.03181 0.41274
C -1.67562 0.87285 2.12977
C -0.95530 2.09750 2.08362
N 0.11437 2.35154 2.92773
C 0.80509 1.29094 3.28795
C 0.51742 -0.02093 2.78424
C -0.88241 -0.28462 2.49674
C -1.50474 -1.57610 2.45695
C -2.85465 -1.69085 2.16026
C -3.66125 -0.53150 1.91720
C -3.08454 0.71855 1.87747
H 1.63031 1.44691 3.99337
H 1.15508 -0.85152 3.09254
H -0.90743 -2.45876 2.69196
H -3.31869 -2.67851 2.13176
H -4.72986 -0.65246 1.73165
H -3.68274 1.60873 1.67098
P 1.63760 1.42435 -0.13708
P -1.40830 0.41354 -1.62031
P 0.97514 -1.97187 -0.30578
C 3.29883 1.09247 0.66885
C 2.19712 1.55090 -1.92375
C 1.52004 3.26434 0.19560
C -0.16495 -3.41485 -0.71485
C 2.12298 -2.12286 -1.79006
C 2.09231 -2.82769 0.94585

C -2.99457 -0.59168 -1.70963
C -2.11985 2.13624 -1.85362
C -0.82687 0.11232 -3.38395
H -1.61734 0.36298 -4.10825
H 0.06577 0.70942 -3.60766
H -0.56832 -0.95026 -3.49315
H -2.78964 2.18624 -2.72601
H -2.67494 2.41543 -0.94797
H -1.29839 2.85389 -1.98797
H -3.59218 -0.29957 -2.58667
H -2.74743 -1.65934 -1.78108
H -3.57896 -0.42967 -0.79461
H 0.40538 -4.35206 -0.80475
H -0.92321 -3.52485 0.07229
H -0.67659 -3.21423 -1.66612
H 2.42590 -3.16947 -1.94631
H 1.61755 -1.75422 -2.69261
H 3.02525 -1.51825 -1.62282
H 2.54717 -3.73881 0.52757
H 2.88721 -2.13756 1.26012
H 1.50289 -3.09591 1.83340
H 4.05520 1.82199 0.34141
H 3.18254 1.15073 1.75857
H 3.63671 0.07942 0.40994
H 3.13776 2.11911 -1.98334
H 2.34177 0.56016 -2.36880
H 1.42997 2.08794 -2.49770
H 2.42972 3.78258 -0.14503
H 0.65083 3.66280 -0.34626
H 1.36743 3.43434 1.26941
H -1.42149 2.97703 1.63017

IV-a

Mo -0.10303 0.37548 0.55502
C -2.02553 0.16090 1.95913
N -1.83771 1.48510 1.52731
C -0.67200 2.07319 1.94671
C 0.39852 1.31183 2.52380
N 0.31469 -0.02740 2.81074
C -0.94345 -0.58956 2.57034
C -1.21181 -1.92340 3.00680
C -2.46306 -2.49091 2.84770
C -3.51597 -1.75747 2.24284
C -3.29479 -0.46225 1.80615
H -0.56144 3.14184 1.75723
H 1.32740 1.81056 2.81031
H -0.40875 -2.45659 3.51915
H -2.64542 -3.50661 3.20421
H -4.50268 -2.20940 2.13203

H -4.10243 0.13484 1.37973
P 1.84023 1.54378 -0.29024
P -1.29736 0.81089 -1.54053
P 0.84211 -1.77417 -0.19437
C 3.48882 0.97381 0.40580
C 2.35143 1.68926 -2.09385
C 1.97424 3.36617 0.13901
C -0.46705 -3.06155 -0.54208
C 1.92420 -2.05312 -1.70369
C 1.89185 -2.67494 1.06152
C -3.09545 0.28907 -1.58476
C -1.53791 2.62374 -1.93127
C -0.80777 0.17218 -3.23670
H -1.48630 0.56015 -4.01182
H 0.22118 0.46488 -3.47868
H -0.86609 -0.92562 -3.23833
H -2.20949 2.76486 -2.79215
H -1.97224 3.09869 -1.04099
H -0.57074 3.09818 -2.14452
H -3.55615 0.53489 -2.55366
H -3.17668 -0.79056 -1.40097
H -3.62478 0.81945 -0.78350
H -0.01307 -4.04372 -0.74438
H -1.13615 -3.13237 0.32571
H -1.06192 -2.75097 -1.41210
H 2.15363 -3.12293 -1.82505
H 1.41164 -1.69029 -2.60416
H 2.86882 -1.50258 -1.59591
H 2.15960 -3.68229 0.70814
H 2.80604 -2.09620 1.24909
H 1.33982 -2.74226 2.00620
H 4.30886 1.64516 0.10822
H 3.41927 0.93659 1.50138
H 3.71146 -0.04058 0.04748
H 3.30852 2.22549 -2.18350
H 2.45624 0.69130 -2.53817
H 1.58534 2.24184 -2.65467
H 2.91741 3.79184 -0.23530
H 1.12913 3.90806 -0.30666
H 1.93402 3.50028 1.22812

IV-b

Mo -0.29464 -0.15566 0.62620
C -1.18444 1.48490 2.16908
N -1.55281 2.78494 1.97015
C -0.63641 3.71735 2.21858
C 0.67913 3.39394 2.63084
N 1.09638 2.14679 2.80595
C 0.17135 1.14729 2.58893

C 0.53015 -0.22692 2.80056
C -0.44706 -1.24266 2.62810
C -1.78262 -0.92441 2.21525
C -2.11671 0.41760 1.89838
H -0.93372 4.76108 2.07924
H 1.40845 4.19088 2.81326
H 1.53763 -0.46145 3.14262
H -0.18290 -2.27768 2.85164
H -2.52816 -1.71036 2.10003
H -3.12515 0.68736 1.58133
P 1.85409 0.54353 -0.35996
P -1.58221 0.58228 -1.33144
P -0.05558 -2.39431 -0.26228
C 3.34981 0.47167 0.75990
C 2.62965 -0.17958 -1.91040
C 1.91800 2.35033 -0.84435
C -1.32511 -3.67290 0.26341
C -0.03606 -2.82688 -2.09006
C 1.49413 -3.32399 0.25158
C -3.21584 -0.29871 -1.59486
C -2.19813 2.35060 -1.29402
C -0.97683 0.57985 -3.11214
H -1.76470 0.93654 -3.79331
H -0.10816 1.24701 -3.20227
H -0.67024 -0.42886 -3.41501
H -2.86794 2.55412 -2.14364
H -2.71620 2.54263 -0.34559
H -1.33710 3.03181 -1.34279
H -3.78954 0.15436 -2.41807
H -3.03261 -1.35794 -1.82152
H -3.80299 -0.24450 -0.66842
H -1.08274 -4.66154 -0.15434
H -1.35587 -3.75029 1.35818
H -2.31812 -3.36362 -0.08983
H 0.14529 -3.90332 -2.23116
H -1.00585 -2.57144 -2.53842
H 0.74823 -2.25953 -2.60639
H 1.48911 -4.36189 -0.11555
H 2.38153 -2.80798 -0.13900
H 1.56112 -3.32429 1.34810
H 4.24360 0.87509 0.25953
H 3.13261 1.05736 1.66424
H 3.53490 -0.57156 1.05129
H 3.56507 0.34594 -2.15648
H 2.85558 -1.24405 -1.75935
H 1.93342 -0.08839 -2.75448
H 2.93839 2.64446 -1.13372
H 1.23754 2.53212 -1.68720
H 1.59113 2.96476 0.00482

IV-IM

Mo -0.21435 -0.41487 0.21439
C -1.01517 1.26974 3.19207
N 0.20783 1.01517 3.78630
C 0.77109 -0.13664 3.43923
C 0.21439 -1.10144 2.56085
N -1.04453 -0.89973 1.98966
C -1.64256 0.33683 2.29434
C -2.88249 0.65002 1.69488
C -3.49605 1.88144 1.94602
C -2.89110 2.79473 2.82484
C -1.67593 2.48852 3.44446
H 1.74273 -0.35922 3.89785
H 0.57883 -2.12853 2.58077
H -3.36117 -0.11310 1.07870
H -4.45135 2.12060 1.47648
H -3.37555 3.75082 3.03153
H -1.19572 3.19032 4.12875
P 0.99218 1.61057 -0.13406
P -1.38222 -0.45534 -1.89225
P 1.52611 -1.89916 -0.38784
C 2.21598 2.13203 1.18544
C 2.08687 1.87713 -1.63590
C -0.03548 3.17831 -0.23025
C 1.13066 -3.71236 -0.08182
C 2.17756 -2.05181 -2.14083
C 3.17151 -1.79352 0.51029
C -2.13518 -2.11255 -2.36616
C -2.93156 0.60200 -2.00021
C -0.63113 0.01406 -3.54666
H -1.32246 -0.23245 -4.36671
H -0.44176 1.09601 -3.55499
H 0.31952 -0.50955 -3.70507
H -3.39598 0.51669 -2.99467
H -3.65224 0.27510 -1.23962
H -2.67460 1.65083 -1.80285
H -2.81135 -2.02558 -3.23088
H -1.33008 -2.82070 -2.60701
H -2.69197 -2.50793 -1.50499
H 1.98371 -4.35997 -0.33682
H 0.87134 -3.85840 0.97590
H 0.26035 -3.99819 -0.68796
H 3.00938 -2.77083 -2.18518
H 1.37174 -2.40203 -2.80010
H 2.52770 -1.07519 -2.50049
H 3.82630 -2.64085 0.25513
H 3.67090 -0.85517 0.23204
H 2.99464 -1.77918 1.59363

H 2.67130 3.10272 0.93619
H 1.70617 2.20417 2.15556
H 3.00256 1.36975 1.26685
H 2.48485 2.90344 -1.64675
H 2.92876 1.17191 -1.59648
H 1.52412 1.69858 -2.56085
H 0.60051 4.07694 -0.22854
H -0.63619 3.16073 -1.15017
H -0.71770 3.21626 0.63026

IV-TS1

Mo 0.27212 -0.10076 0.23548
C -1.81588 1.17598 2.22375
N -0.50484 1.66391 2.08304
C 0.47919 0.77523 2.46092
C 0.29891 -0.62658 2.39003
N -0.88927 -0.94626 1.66412
C -2.04563 -0.21723 2.07043
C -3.32141 -0.76543 2.18175
C -4.41459 0.08317 2.44133
C -4.20490 1.46019 2.58292
C -2.91584 2.00933 2.48111
H 1.41219 1.19039 2.85546
H 0.89281 -1.38782 2.89937
H -3.45973 -1.84029 2.04479
H -5.42085 -0.33191 2.51522
H -5.05381 2.12052 2.77214
H -2.75022 3.08303 2.58940
P 1.75582 1.84602 -0.13303
P -1.30804 0.10030 -1.62029
P 1.64707 -1.98413 -0.29960
C 3.19896 2.29352 0.97127
C 2.66036 1.64653 -1.75828
C 0.96720 3.52303 -0.31008
C 0.79449 -3.61933 0.00844
C 2.30632 -2.26172 -2.03095
C 3.23378 -2.25825 0.66628
C -2.41869 -1.39016 -1.84195
C -2.60373 1.43873 -1.44500
C -0.81375 0.38923 -3.40710
H -1.69626 0.39183 -4.06546
H -0.30578 1.36031 -3.49224
H -0.12067 -0.39842 -3.73318
H -3.35806 1.37597 -2.24433
H -3.09399 1.33514 -0.46733
H -2.11558 2.42218 -1.47569
H -3.21139 -1.19193 -2.57978
H -1.81555 -2.24680 -2.17218
H -2.87252 -1.63603 -0.87236

H 1.48500 -4.46241 -0.14565
H 0.41542 -3.62827 1.03887
H -0.06344 -3.71149 -0.66984
H 2.93914 -3.16155 -2.07283
H 1.45826 -2.37801 -2.71877
H 2.89985 -1.39563 -2.35382
H 3.70944 -3.21961 0.41715
H 3.93098 -1.43877 0.44220
H 3.00784 -2.22959 1.74055
H 3.83071 3.06100 0.49906
H 2.81834 2.68940 1.92217
H 3.79638 1.39534 1.17652
H 3.12642 2.60148 -2.04295
H 3.44595 0.88734 -1.64823
H 1.96887 1.33260 -2.55052
H 1.71747 4.32073 -0.42041
H 0.30259 3.51236 -1.18460
H 0.35626 3.68469 0.58904

IV-TS2

Mo -0.27250 -0.06668 0.31233
C -1.22709 1.19633 2.74866
N -0.35499 2.00326 3.39901
C 0.82984 1.43749 3.70585
C 1.17668 0.13351 3.31389
N 0.32962 -0.73849 2.71582
C -0.93332 -0.20417 2.46532
C -1.96878 -1.08131 1.99300
C -3.17633 -0.53402 1.59611
C -3.45065 0.86115 1.78526
C -2.51350 1.69249 2.36347
H 1.54793 2.05318 4.25373
H 2.17938 -0.24895 3.53242
H -1.77582 -2.15345 1.94886
H -3.95847 -1.18255 1.19794
H -4.42320 1.25673 1.48863
H -2.72804 2.74373 2.56544
P 1.38448 1.49534 -0.30320
P -1.44287 0.00116 -1.76434
P 0.99858 -1.97747 -0.22735
C 3.08203 1.43841 0.50685
C 1.96379 1.83139 -2.06173
C 0.90449 3.25728 0.15931
C 0.09251 -3.61858 -0.43403
C 2.06163 -2.05700 -1.77388
C 2.29596 -2.53979 1.00292
C -2.93896 -1.12841 -1.95651
C -2.30047 1.64257 -2.10881

C -0.70979 -0.30983 -3.46678
H -1.43382 -0.03323 -4.24801
H 0.21330 0.26459 -3.60622
H -0.47875 -1.37913 -3.56766
H -2.97929 1.56881 -2.97286
H -2.87469 1.93946 -1.21969
H -1.54572 2.41632 -2.30521
H -3.38964 -1.02902 -2.95613
H -2.63420 -2.17162 -1.79778
H -3.68630 -0.86582 -1.19701
H 0.78861 -4.45254 -0.61482
H -0.48421 -3.82717 0.47816
H -0.60782 -3.54400 -1.27778
H 2.51757 -3.05311 -1.88081
H 1.46781 -1.83597 -2.66863
H 2.86141 -1.30786 -1.69342
H 2.80095 -3.45231 0.65155
H 3.03868 -1.74195 1.13796
H 1.80524 -2.72049 1.96699
H 3.68500 2.32148 0.24426
H 2.95691 1.39328 1.59645
H 3.60907 0.53203 0.17707
H 2.74289 2.60895 -2.07199
H 2.36716 0.91443 -2.51166
H 1.11380 2.17536 -2.66697
H 1.69939 3.97208 -0.10525
H -0.01834 3.53226 -0.37074
H 0.71008 3.30839 1.23988

V

C -1.13471 1.12880 2.28251
C -1.53022 -0.21441 2.52068
C -0.52475 -1.23059 2.60671
C 0.85433 -0.89418 2.55438
C 1.26501 0.48775 2.49219
C 0.25696 1.52526 2.37410
H -2.58742 -0.47217 2.57531
H -0.81586 -2.27194 2.75499
H 1.61112 -1.67267 2.65654
H -1.89467 1.90920 2.20359
Mo -0.20707 -0.13810 0.63158
P -1.29412 1.36993 -0.95661
P -1.33770 -2.03987 -0.32593
P 1.73401 -0.46187 -0.83975
C -0.43509 -3.68693 -0.20414
C -2.95733 -2.56511 0.46930
C -1.90553 -2.19871 -2.11280
C -0.99335 3.21394 -0.74738
C -1.09504 1.33041 -2.82847

C -3.17029 1.40692 -0.88693
H -3.34754 -3.48250 0.00327
H -2.81054 -2.74843 1.54195
H -3.69446 -1.75881 0.35475
H -1.05608 -4.52460 -0.55800
H 0.48589 -3.64530 -0.80185
H -0.14998 -3.85897 0.84290
H -2.34809 -3.19043 -2.29307
H -2.66104 -1.43188 -2.33192
H -1.05731 -2.05614 -2.79423
H -3.58588 2.19667 -1.53222
H -3.57293 0.43485 -1.20217
H -3.48210 1.58204 0.15183
H -1.52623 3.79398 -1.51633
H -1.34289 3.53006 0.24387
H 0.08321 3.42134 -0.81130
H -1.74882 2.07423 -3.30948
H -0.05224 1.56131 -3.08806
H -1.33655 0.33414 -3.21896
C 3.14185 -1.51410 -0.18370
C 1.68264 -1.19691 -2.57020
C 2.68397 1.10245 -1.23423
H 2.68211 -1.17804 -3.03147
H 1.33882 -2.23949 -2.52167
H 0.98533 -0.63048 -3.20039
H 3.61058 0.88204 -1.78656
H 2.05330 1.76966 -1.83778
H 2.92610 1.61637 -0.29429
H 3.98013 -1.55251 -0.89621
H 3.49538 -1.09225 0.76529
H 2.77590 -2.53290 0.00345
C 2.63656 0.89154 2.57953
C 3.00142 2.22455 2.55056
H 3.39673 0.11987 2.72179
H 4.05413 2.50107 2.63749
C 2.01548 3.23607 2.41900
H 2.30910 4.28662 2.39921
C 0.67958 2.88551 2.32398
H -0.08381 3.66371 2.25537

V-IM

C -1.93415 1.17314 3.38551
C -2.51224 -0.09554 3.33374
C -1.76848 -1.21080 2.90717
C -0.41955 -1.07509 2.51594
C 0.20569 0.22903 2.57104
C -0.58828 1.38251 2.98905
H -3.55158 -0.23050 3.63861
H -2.22680 -2.20157 2.91591

H 0.21660 -1.96382 2.44545
Mo 0.19749 -0.20119 0.32277
P -0.99715 1.35385 -0.97908
P -0.80098 -2.11885 -0.67424
P 2.13059 -0.20893 -1.06026
C -0.29070 -3.77326 0.07078
C -2.66684 -2.28842 -0.49489
C -0.70113 -2.63591 -2.48162
C -0.41392 3.13037 -0.80421
C -1.24924 1.32167 -2.84229
C -2.78802 1.57257 -0.45509
H -2.99627 -3.30875 -0.74540
H -2.96499 -2.04132 0.53178
H -3.15911 -1.58158 -1.17751
H -0.79584 -4.61279 -0.43103
H 0.79703 -3.89513 -0.03044
H -0.54462 -3.79261 1.13939
H -1.39914 -3.46443 -2.67630
H -0.95412 -1.78977 -3.13329
H 0.31482 -2.96953 -2.72469
H -3.24844 2.42476 -0.97826
H -3.35680 0.66119 -0.67966
H -2.82537 1.74499 0.62934
H -1.12182 3.82511 -1.28192
H -0.32403 3.37336 0.26330
H 0.57348 3.24348 -1.26944
H -1.83918 2.18620 -3.18449
H -0.27056 1.33395 -3.34208
H -1.77260 0.39743 -3.12397
C 3.62299 -1.12344 -0.35786
C 2.24596 -0.89493 -2.80873
C 2.95616 1.44694 -1.40695
H 3.20805 -0.61457 -3.26411
H 2.17843 -1.99003 -2.78218
H 1.42518 -0.50790 -3.42596
H 3.96452 1.30668 -1.82641
H 2.34729 2.00614 -2.13122
H 3.01580 2.03268 -0.48100
H 4.47134 -1.10517 -1.05908
H 3.93389 -0.65707 0.58702
H 3.34574 -2.16777 -0.15563
C 1.59461 0.41386 2.20921
C 2.13618 1.71633 2.22579
H 2.26119 -0.45300 2.18577
H 3.19037 1.85991 1.98114
C 1.36141 2.82060 2.63421
H 1.81672 3.81247 2.65561
C 0.03647 2.65764 3.03256
H -0.54788 3.51620 3.37083

H -2.51817 2.03066 3.72734

V-TS

C -1.88401 1.22870 3.37339
C -2.50175 -0.01899 3.29514
C -1.78616 -1.15467 2.87110
C -0.42490 -1.06255 2.51086
C 0.23300 0.22537 2.56856
C -0.52715 1.39883 2.99344
H -3.55028 -0.12394 3.57982
H -2.27573 -2.13045 2.86824
H 0.18603 -1.96950 2.45971
Mo 0.20047 -0.21120 0.32117
P -1.05061 1.32112 -0.95011
P -0.77587 -2.14488 -0.66711
P 2.11097 -0.16621 -1.09763
C -0.28713 -3.78559 0.12247
C -2.64608 -2.31588 -0.54150
C -0.61595 -2.69500 -2.46018
C -0.49822 3.10788 -0.77459
C -1.32589 1.29055 -2.80996
C -2.83786 1.50621 -0.40215
H -2.96604 -3.34222 -0.77946
H -2.97588 -2.04719 0.46999
H -3.11817 -1.62523 -1.25432
H -0.76849 -4.63529 -0.38557
H 0.80427 -3.90348 0.06533
H -0.58250 -3.79049 1.18057
H -1.31357 -3.52100 -2.66650
H -0.83388 -1.85857 -3.13649
H 0.40581 -3.04373 -2.65497
H -3.31885 2.35386 -0.91405
H -3.39353 0.58662 -0.62554
H -2.86399 1.67085 0.68374
H -1.22613 3.79119 -1.23848
H -0.39789 3.34817 0.29273
H 0.48005 3.24308 -1.25313
H -1.95121 2.13473 -3.14001
H -0.35486 1.34141 -3.32206
H -1.81825 0.34878 -3.08982
C 3.61291 -1.10280 -0.44798
C 2.20690 -0.78049 -2.87394
C 2.92516 1.50544 -1.38960
H 3.16407 -0.48065 -3.32729
H 2.13792 -1.87519 -2.89525
H 1.38023 -0.36698 -3.46587
H 3.92932 1.38534 -1.82505
H 2.30644 2.08914 -2.08561
H 2.99249 2.05574 -0.44270

H	4.45602	-1.04959	-1.15378
H	3.92799	-0.67693	0.51444
H	3.34177	-2.15631	-0.29007
C	1.62470	0.37611	2.20161
C	2.21200	1.65773	2.25177
H	2.26178	-0.51252	2.15324
H	3.27088	1.77086	2.01145
C	1.47146	2.77850	2.67497
H	1.95805	3.75466	2.71773
C	0.13722	2.65195	3.05802
H	-0.42273	3.52425	3.40256
H	-2.44432	2.10048	3.71869