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Supporting info

Conformational Studies of Template-Assisted Self-Assembled Molecular Capsules and the Use of their Rhodium Complexes in Hydroformylation reactions†

Ivo Jacobs,^a Adri C. T. van Duin,^b Arjan W. Kleij,^{a,d} Mark Kuil,^a Duncan M. Tooke,^c Anthony L. Spek^c and Joost N. H. Reek^{*a}

Detailed Results of Hydroformylation Catalysis

Table S1. A summary of the results of octene hydroformylation using supramolecular rhodium catalysts based on the tris-*m*-pyridylphosphine template.

Entry	Substrate ¹	Building block ²	Substrate: catalyst ratio	Reaction time	out/in	Yield	TOF	Ref.
1	1	-	1052	65	2.30	31	5	1
2	1	2f	1052	65	1.40	97	16	1
3	1	2c	1052	65	1.00	97	16	1
4	1	2b	1052	65	1.20	97	16	1
5	1	2d	1052	65	0.80	97	16	1
6	1	-	1052	24	2.88	6	3	2
7	1	2a	1052	24	0.56	52	23	2
8	2	-	1052	73	1.27	17	2	2
9	2	2a	1052	73	0.11	32	5	2
10	2	2c	1052	73	1.04	47	7	3
11	2	2d	1052	73	0.86	48	7	3
12	3	-	1052	73	0.98	26	4	2
13	3	2a	1052	73	0.31	45	6	2
14	3	2c	1052	73	1.03	60	9	3
15	3	2d	1052	73	0.98	63	9	3
16	1	-	5160	18	2.80	4	11	4
17	1	2a	5160	18	0.60	44	126	4
18	1	-	1000	16	2.50	27	16	5
19	1	2b	1000	16	1.60	59	38	5
20	1	2c	1000	16	1.30	42	27	5
21	1	2e	1000	16	1.90	22	13	5
22	1	2f	1000	16	1.80	21	12	5

References

- 1 AW Kleij, M Lutz, AL Spek, PWNM van Leeuwen, JNH Reek, Chem Commun, 2005 (29) pp. 3661-3663.
- 2 M Kuil, T Soltner, PWNM van Leeuwen, JNH Reek, J Am Chem Soc, 2006 vol. 128 (35) pp. 11344-11345.
- 3 M Kuil, PhD Thesis, University of Amsterdam.
- 4 VF Slagt, JNH Reek, PCJ Kamer, PWNM van Leeuwen, Angew. Chem. Int. Edit., 2001 vol. 40 (22) pp. 4271-4274.
- 5 This paper.

¹ 1: 1-octene, 2: 2-octene, 3: 3-octene.

² See Scheme 1 in the main article.

Raw NMR data

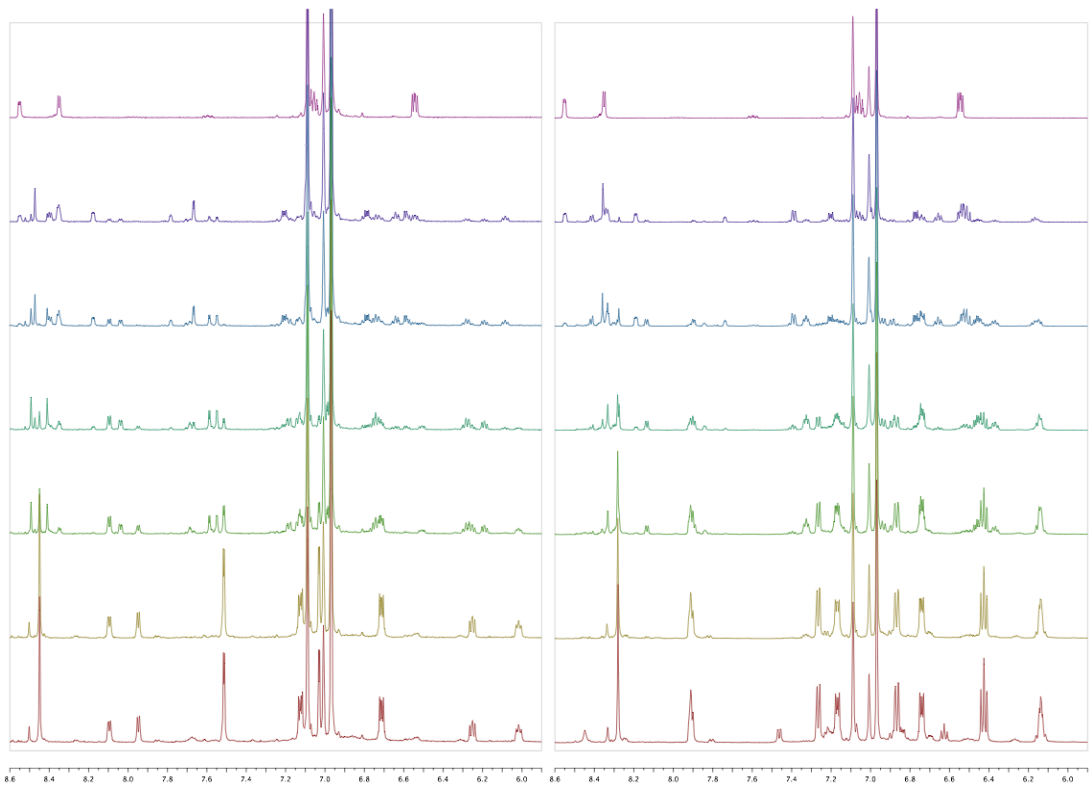


Figure S1. Aromatic regions of the spectra in Fig. 7

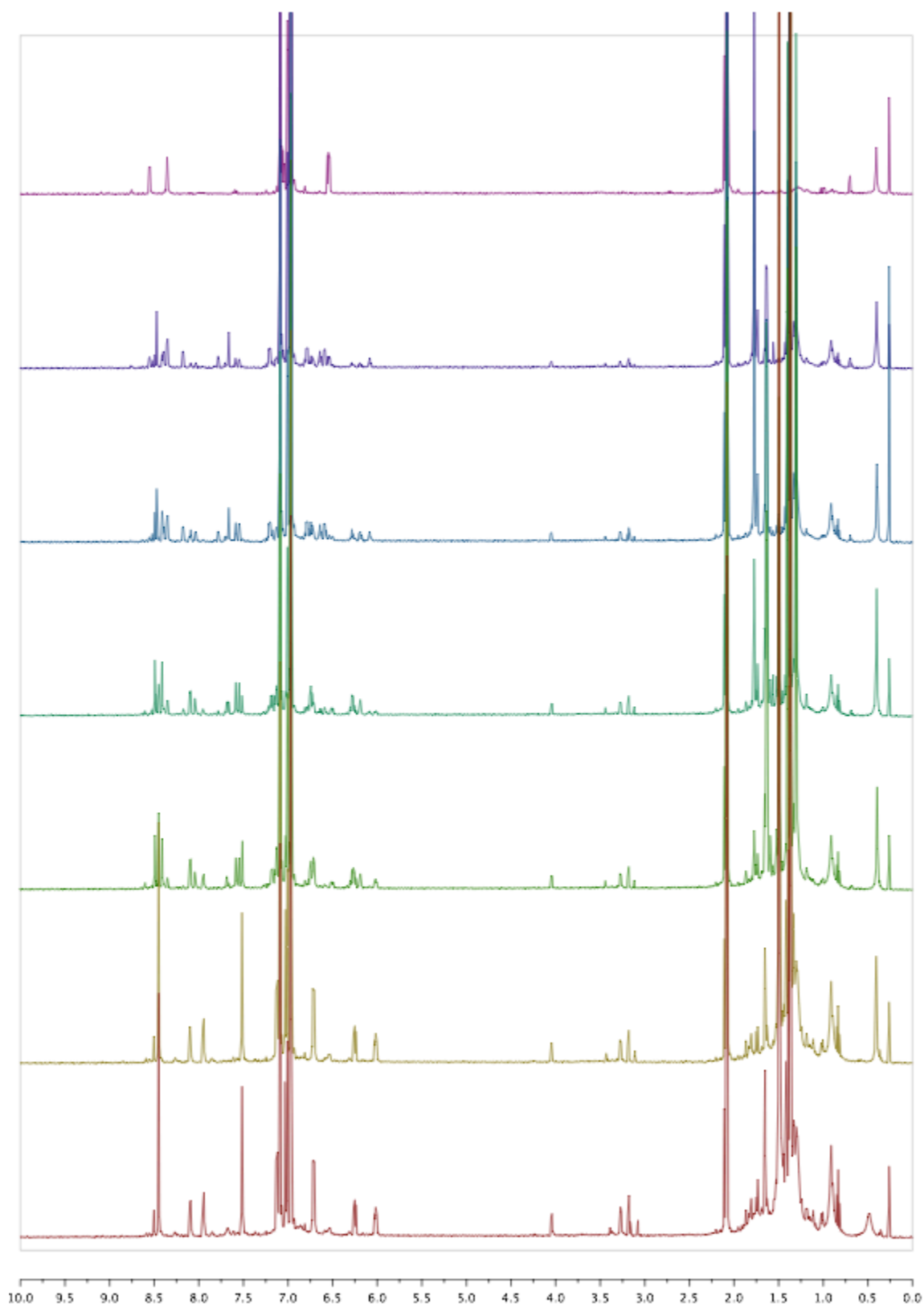


Figure S2. Full spectra of the NMR titration of **1** with **2j** in figure 7

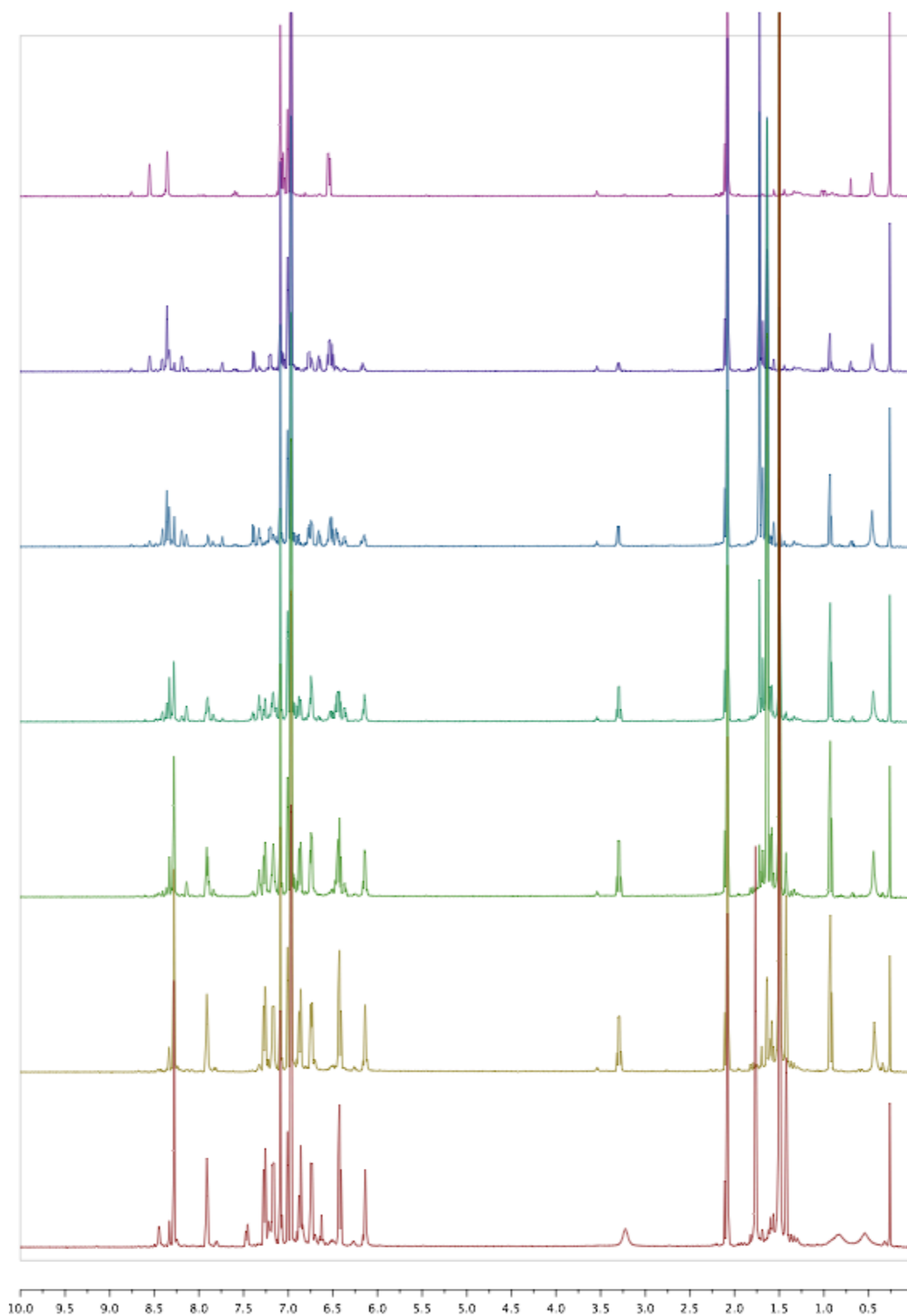


Figure S3. Full spectra of the NMR titration of **1** with **2i** in figure 7

Results of DFT calculations used for Ru- and Zn-parametrization

DFT calculations were performed with Jaguar³ using the B3LYP functional and the 6-31G**++ basis set.

Pyridine:

11

N13	1.3932312687	0.0105087118	0.0000000000
C14	0.6861595955	1.1495270907	0.0000000000
C15	-0.7103469593	1.1941248964	0.0000000000
C16	-1.4147239507	-0.0109316183	0.0000000000
C17	-0.6924766870	-1.2048734699	0.0000000000
C18	0.7036495111	-1.1386093907	0.0000000000
H19	1.2661341870	2.0700946284	0.0000000000
H20	-1.2271455990	2.1488665324	0.0000000000
H21	-2.5009957992	-0.0182948298	0.0000000000
H22	-1.1934222425	-2.1680063101	0.0000000000
H23	1.2972238117	-2.0505245992	0.0000000000

energy: -248.30339650304 hartrees

Ru(II)Salen-CO:

23

Ru1	-0.0500382455	0.1638954460	0.0875980600
O1	-0.1760349604	-0.0741442648	2.1704778235
C2	0.8698524838	-0.1195987989	2.9020075584
C3	2.2219928672	-0.1279101689	2.5134654804
C4	2.7256419122	-0.1326920759	1.2045316114
N5	1.9867186014	-0.0554638595	0.1030229912
C6	2.5200297882	-0.1069829223	-1.1831576418
C7	1.6450636099	-0.1062531313	-2.2248501053
N8	0.2862229051	-0.0541411903	-1.9215865065
C9	-0.6711272862	-0.1315354341	-2.8395141240
C10	-2.0472555488	-0.1274708603	-2.5692704645
C11	-2.6633706598	-0.1196653212	-1.3044834585
O12	-2.1235702437	-0.0736398874	-0.1479587168
H24	0.6730792053	-0.1806091508	3.9801653035
H25	2.9485547802	-0.1849618837	3.3171204868
H26	3.8069538375	-0.2297397018	1.0738449111
H27	3.5976726138	-0.1510654854	-1.3156545747
H28	1.9616657163	-0.1496629488	-3.2634651289
H29	-0.3557767032	-0.2273231025	-3.8821500593
H30	-2.7135899374	-0.1845389864	-3.4235255784
H31	-3.7592985573	-0.1818490343	-1.2968746687

³ Jaguar, version 7.0, Schrodinger, LLC, New York, NY, 2007.

C32	-0.0287185904	1.9743924188	0.0704335630
O33	-0.0094580043	3.1377616798	0.0546231807

energy: -776.92927488154 hartrees

Ru(II)Salen-CO-Pyridine:

34

Ru1	-0.0231188138	0.0876492671	0.0603906404
O1	-0.1236775819	-0.1448427033	2.1749449313
C2	0.9481483319	-0.1572672672	2.8678756385
C3	2.2898264759	-0.0674509318	2.4532181730
C4	2.7834642481	0.0523109276	1.1402585737
N5	2.0368384906	0.1175374854	0.0510002610
C6	2.5491997426	0.2272988747	-1.2383621870
C7	1.6636306989	0.2375710000	-2.2751674043
N8	0.3088191649	0.1378908548	-1.9718490551
C9	-0.6510310810	0.0909321570	-2.8803482771
C10	-2.0262051851	-0.0193800310	-2.5991685018
C11	-2.6461174158	-0.1172855274	-1.3398065147
O12	-2.1289245795	-0.1211993648	-0.1730663704
N13	-0.0044410927	-2.1402851162	0.0232633748
C14	-0.9102377644	-2.7742802314	0.7922068619
C15	-0.9896055081	-4.1643634813	0.8583940162
C16	-0.1008945820	-4.9300597233	0.1029335138
C17	0.8373262131	-4.2722597519	-0.6941313664
C18	0.8521417946	-2.8789111987	-0.7055721244
H19	-1.5765375787	-2.1333303443	1.3585898064
H20	-1.7370715268	-4.6289715383	1.4929948064
H21	-0.1380980807	-6.0151387835	0.1340374655
H22	1.5494735460	-4.8231283998	-1.2997712222
H23	1.5634762899	-2.3269233385	-1.3103912099
H24	0.7917479024	-0.2601727752	3.9509989242
H25	3.0294816281	-0.1041319718	3.2465264338
H26	3.8691955540	0.0883205517	1.0081892635
H27	3.6242541142	0.3007504256	-1.3844064509
H28	1.9765624107	0.3194834791	-3.3134436969
H29	-0.3503140953	0.1353434782	-3.9317656765
H30	-2.6942147444	-0.0413300429	-3.4542343454
H31	-3.7412244686	-0.2107015160	-1.3555961497
C32	-0.1330592876	1.9557144391	0.1754676105
O33	-0.2090428902	3.1097289792	0.2542945733

energy: -1025.25992590245 hartrees

Zn(II)Salen:

21

Zn1	-0.3300311178	0.2751305970	0.0000000000
O1	-0.3514036433	2.2593814459	0.0000000000
C2	0.6741227692	3.0289444490	0.0000000000
C3	2.0260858372	2.6688755872	0.0000000000
C4	2.5154530464	1.3497655263	0.0000000000
N5	1.7486934519	0.2729922676	0.0000000000
C6	2.2635741869	-1.0106073289	0.0000000000
C7	1.3879351027	-2.0537194992	0.0000000000
N8	0.0343971802	-1.7684865102	0.0000000000
C9	-0.8942865096	-2.7093086342	0.0000000000
C10	-2.2781288010	-2.4548665632	0.0000000000
C11	-2.8674963548	-1.1861320086	0.0000000000
O12	-2.2882605402	-0.0419760384	0.0000000000
H24	0.4495376666	4.1047384620	0.0000000000
H25	2.7510791060	3.4756740838	0.0000000000
H26	3.6029299924	1.2076646550	0.0000000000
H27	3.3417541468	-1.1633683812	0.0000000000
H28	1.7244683550	-3.0893042430	0.0000000000
H29	-0.5669276418	-3.7559521964	0.0000000000
H30	-2.9472675071	-3.3085831430	0.0000000000
H31	-3.9659733368	-1.1520401867	0.0000000000

energy: -2349.12268838303 hartrees

Zn(II)Salen-Pyridine:

32

Zn1	-0.0570398574	-0.2052107547	0.0885031933
O1	-0.1884238762	-0.0358838025	2.1213307897
C2	0.7815237355	0.1821954309	2.9274034821
C3	2.1322396515	0.3921440207	2.6279484990
C4	2.6819464569	0.4710967814	1.3310807940
N5	1.9915629939	0.3175422201	0.2184228078
C6	2.5620782473	0.4793881996	-1.0315535042
C7	1.7531981792	0.4293060140	-2.1280229500
N8	0.3996184047	0.2159166188	-1.9383005890
C9	-0.4785780521	0.3157129057	-2.9194991693
C10	-1.8742584776	0.2391842829	-2.7468134045
C11	-2.5359414472	0.1589623871	-1.5110592144
O12	-2.0303922490	0.0611374666	-0.3442611404
N13	-0.0827857972	-2.3879833990	0.0638637282
C14	-0.4132865814	-3.0581742963	1.1813431128
C15	-0.4706147111	-4.4513239125	1.2271578546
C16	-0.1766750754	-5.1744004169	0.0699207496
C17	0.1594089101	-4.4773628976	-1.0924812366
C18	0.1936463361	-3.0843805734	-1.0516449819
H19	-0.6353147652	-2.4441187578	2.0490184925
H20	-0.7409240823	-4.9515102697	2.1517868991
H21	-0.2112764139	-6.2602827173	0.0727417970

H22	0.3912641065	-4.9971564881	-2.0164914711
H23	0.4469665484	-2.4978134877	-1.9295680713
H24	0.5123268515	0.2088215842	3.9951786606
H25	2.8017962485	0.5510199869	3.4668541235
H26	3.7535846815	0.6956327093	1.2487866294
H27	3.6308032212	0.6764721268	-1.1188945174
H28	2.1426203147	0.5894736961	-3.1336290480
H29	-0.1017198395	0.4976676235	-3.9350005286
H30	-2.4959532130	0.3244597762	-3.6321225263
H31	-3.6360654841	0.2014697992	-1.5496830738

energy: -2597.44228629196 hartrees

Details of ReaxFF simulations

Initial structures for the in and out conformations of Zn-complex **3b** were recovered from the X-ray crystal structure. The corresponding structures for Ru-complex **3g** were constructed by replacing the zinc atoms for ruthenium, and adding the three carbon monoxide ligands. The simulations were performed under periodic boundary conditions, using a cubic box with a length of 80 Å. An NVT regime was used. The initial structures were equilibrated at 250 K before starting the drives. The resulting structures are presented below. These were used as the starting points for the drives.

For the ruthenium complexes the following bond constraints were used during all simulations to keep the CO-ligands attached:

BOND RESTRAINT 1 221 1.9000 1500.00 0.0500 0.0000000

BOND RESTRAINT 75 223 1.9000 1500.00 0.0500 0.0000000

BOND RESTRAINT 148 225 1.9000 1500.00 0.0500 0.0000000

The first two numbers identify the centers concerned, the third one the equilibrium bond length R12, the fourth and fifth are Force1 and Force2 in the following formula:

$$E_{restraint} = Force1 * \{1.0 - \exp(Force2 * (R_{ij} - R12)^2)\}$$

The final number is the change in bond length per iteration.

Structures

3b-in:

HETATM	1 Zn	5.26700	2.35600	3.37300	Zn	1 0	0.00000
HETATM	2 P	0.00000	0.00000	3.42000	P_3	1 0	0.00000
HETATM	3 O	5.73800	0.56300	3.96500	O_3	2 0	0.00000
HETATM	4 O	6.38700	2.33800	1.76500	O_3	2 0	0.00000
HETATM	5 N	3.34800	2.09600	2.48400	N_R	2 0	0.00000
HETATM	6 N	4.51200	2.76500	5.28100	N_2	3 0	0.00000
HETATM	7 N	5.34500	4.42900	3.40000	N_2	3 0	0.00000
HETATM	8 C	1.11500	1.20500	2.57400	C_R	3 0	0.00000
HETATM	9 C	0.74700	2.03500	1.53400	C_R	3 0	0.00000
HETATM	10 C	1.68200	2.88700	0.98500	C_R	3 0	0.00000
HETATM	11 C	2.97600	2.88200	1.46600	C_R	3 0	0.00000
HETATM	12 C	2.42700	1.29000	3.01600	C_R	3 0	0.00000
HETATM	13 C	4.21600	4.13200	5.48400	C_R	3 0	0.00000
HETATM	14 C	4.65400	5.01400	4.48300	C_R	3 0	0.00000
HETATM	15 C	4.37500	6.37800	4.61400	C_R	3 0	0.00000
HETATM	16 C	3.71200	6.87000	5.72200	C_R	3 0	0.00000
HETATM	17 C	3.28700	5.99700	6.71000	C_R	3 0	0.00000
HETATM	18 C	3.52400	4.65100	6.58200	C_R	3 0	0.00000
HETATM	19 C	4.26600	1.84500	6.16400	C_3	4 0	0.00000
HETATM	20 C	4.51300	0.43400	6.00300	C_R	3 0	0.00000
HETATM	21 C	3.99700	-0.38500	7.03700	C_R	3 0	0.00000
HETATM	22 C	4.14200	-1.74200	6.97500	C_R	3 0	0.00000
HETATM	23 C	4.79800	-2.30400	5.89200	C_R	3 0	0.00000
HETATM	24 C	5.35400	-1.59000	4.86600	C_R	3 0	0.00000
HETATM	25 C	5.20600	-0.14100	4.90700	C_R	3 0	0.00000
HETATM	26 C	5.97000	5.14100	2.52100	C_3	4 0	0.00000
HETATM	27 C	6.72700	4.67300	1.38700	C_R	3 0	0.00000

HETATM	28 C	6.93800	3.28300	1.08000	C_R	3 0	0.00000
HETATM	29 C	7.81000	2.96000	-0.02400	C_R	3 0	0.00000
HETATM	30 C	8.36800	3.98800	-0.73700	C_R	3 0	0.00000
HETATM	31 C	8.14500	5.34100	-0.45700	C_R	3 0	0.00000
HETATM	32 C	7.34400	5.67400	0.59700	C_R	3 0	0.00000
HETATM	33 C	6.08000	-2.25500	3.69400	C_3	4 0	0.00000
HETATM	34 C	7.52600	-1.80000	3.62100	C_3	4 0	0.00000
HETATM	35 C	5.33700	-1.91900	2.36500	C_3	4 0	0.00000
HETATM	36 C	6.06100	-3.80200	3.85000	C_3	4 0	0.00000
HETATM	37 C	8.10300	1.49100	-0.36300	C_3	4 0	0.00000
HETATM	38 C	9.07200	1.36200	-1.55400	C_3	4 0	0.00000
HETATM	39 C	8.74800	0.77700	0.84700	C_3	4 0	0.00000
HETATM	40 C	6.81100	0.75000	-0.72800	C_3	4 0	0.00000
HETATM	41 H	-0.14300	2.01800	1.19700	H_	1 0	0.00000
HETATM	42 H	1.43500	3.47600	0.28100	H_	1 0	0.00000
HETATM	43 H	3.62000	3.45100	1.06400	H_	1 0	0.00000
HETATM	44 H	2.68500	0.73700	3.74300	H_	1 0	0.00000
HETATM	45 H	4.64900	6.97800	3.92900	H_	1 0	0.00000
HETATM	46 H	3.54700	7.80200	5.80800	H_	1 0	0.00000
HETATM	47 H	2.83200	6.33000	7.47600	H_	1 0	0.00000
HETATM	48 H	3.20900	4.05800	7.25400	H_	1 0	0.00000
HETATM	49 H	3.88800	2.12700	6.98900	H_	1 0	0.00000
HETATM	50 H	3.54900	0.01100	7.77800	H_	1 0	0.00000
HETATM	51 H	3.79200	-2.29300	7.66700	H_	1 0	0.00000
HETATM	52 H	4.86900	-3.25100	5.86100	H_	1 0	0.00000
HETATM	53 H	5.92800	6.08200	2.63700	H_	1 0	0.00000
HETATM	54 H	8.93800	3.76900	-1.46100	H_	1 0	0.00000
HETATM	55 H	8.54600	6.01700	-0.99000	H_	1 0	0.00000
HETATM	56 H	7.19700	6.59000	0.80500	H_	1 0	0.00000
HETATM	57 H	7.55800	-0.82600	3.52100	H_	1 0	0.00000
HETATM	58 H	7.96300	-2.22100	2.84900	H_	1 0	0.00000
HETATM	59 H	7.99300	-2.06000	4.44200	H_	1 0	0.00000
HETATM	60 H	5.41800	-0.96100	2.17600	H_	1 0	0.00000
HETATM	61 H	4.39100	-2.15600	2.45200	H_	1 0	0.00000
HETATM	62 H	5.73700	-2.43000	1.63100	H_	1 0	0.00000
HETATM	63 H	6.40500	-4.21700	3.02900	H_	1 0	0.00000
HETATM	64 H	5.14400	-4.10300	4.00800	H_	1 0	0.00000
HETATM	65 H	6.62800	-4.06000	4.60700	H_	1 0	0.00000
HETATM	66 H	8.66700	1.76700	-2.35100	H_	1 0	0.00000
HETATM	67 H	9.25300	0.41600	-1.72600	H_	1 0	0.00000
HETATM	68 H	9.91200	1.82300	-1.34500	H_	1 0	0.00000
HETATM	69 H	9.59900	1.21200	1.07000	H_	1 0	0.00000
HETATM	70 H	8.91300	-0.16300	0.62500	H_	1 0	0.00000
HETATM	71 H	8.14300	0.82800	1.61500	H_	1 0	0.00000
HETATM	72 H	6.20400	0.75700	0.04200	H_	1 0	0.00000
HETATM	73 H	7.02200	-0.17500	-0.96900	H_	1 0	0.00000
HETATM	74 H	6.38500	1.19600	-1.48800	H_	1 0	0.00000
HETATM	75 Zn	-4.67400	3.38300	3.37300	Zn	1 0	0.00000
HETATM	76 O	-3.35700	4.68900	3.96500	O_3	2 0	0.00000
HETATM	77 O	-5.21800	4.36200	1.76500	O_3	2 0	0.00000

HETATM	78 N	-3.48900	1.85200	2.48400 N_R	2 0	0.00000
HETATM	79 N	-4.65100	2.52600	5.28100 N_2	3 0	0.00000
HETATM	80 N	-6.50700	2.41400	3.40000 N_2	3 0	0.00000
HETATM	81 C	-1.60100	0.36300	2.57400 C_R	3 0	0.00000
HETATM	82 C	-2.13500	-0.37000	1.53400 C_R	3 0	0.00000
HETATM	83 C	-3.34100	0.01300	0.98500 C_R	3 0	0.00000
HETATM	84 C	-3.98400	1.13700	1.46600 C_R	3 0	0.00000
HETATM	85 C	-2.33100	1.45600	3.01600 C_R	3 0	0.00000
HETATM	86 C	-5.68700	1.58500	5.48400 C_R	3 0	0.00000
HETATM	87 C	-6.66900	1.52300	4.48300 C_R	3 0	0.00000
HETATM	88 C	-7.71100	0.60000	4.61400 C_R	3 0	0.00000
HETATM	89 C	-7.80500	-0.22000	5.72200 C_R	3 0	0.00000
HETATM	90 C	-6.83700	-0.15200	6.71000 C_R	3 0	0.00000
HETATM	91 C	-5.79000	0.72600	6.58200 C_R	3 0	0.00000
HETATM	92 C	-3.73100	2.77200	6.16400 C_3	4 0	0.00000
HETATM	93 C	-2.63200	3.69200	6.00300 C_R	3 0	0.00000
HETATM	94 C	-1.66500	3.65400	7.03700 C_R	3 0	0.00000
HETATM	95 C	-0.56200	4.45800	6.97500 C_R	3 0	0.00000
HETATM	96 C	-0.40400	5.30700	5.89200 C_R	3 0	0.00000
HETATM	97 C	-1.30000	5.43200	4.86600 C_R	3 0	0.00000
HETATM	98 C	-2.48100	4.57900	4.90700 C_R	3 0	0.00000
HETATM	99 C	-7.43700	2.60000	2.52100 C_3	4 0	0.00000
HETATM	100 C	-7.41000	3.48900	1.38700 C_R	3 0	0.00000
HETATM	101 C	-6.31300	4.36700	1.08000 C_R	3 0	0.00000
HETATM	102 C	-6.46800	5.28300	-0.02400 C_R	3 0	0.00000
HETATM	103 C	-7.63700	5.25300	-0.73700 C_R	3 0	0.00000
HETATM	104 C	-8.69800	4.38400	-0.45700 C_R	3 0	0.00000
HETATM	105 C	-8.58600	3.52300	0.59700 C_R	3 0	0.00000
HETATM	106 C	-1.08700	6.39300	3.69400 C_3	4 0	0.00000
HETATM	107 C	-2.20400	7.41700	3.62100 C_3	4 0	0.00000
HETATM	108 C	-1.00700	5.58200	2.36500 C_3	4 0	0.00000
HETATM	109 C	0.26200	7.15000	3.85000 C_3	4 0	0.00000
HETATM	110 C	-5.34200	6.27200	-0.36300 C_3	4 0	0.00000
HETATM	111 C	-5.71600	7.17500	-1.55400 C_3	4 0	0.00000
HETATM	112 C	-5.04700	7.18800	0.84700 C_3	4 0	0.00000
HETATM	113 C	-4.05500	5.52400	-0.72800 C_3	4 0	0.00000
HETATM	114 H	-1.67600	-1.13300	1.19700 H_	1 0	0.00000
HETATM	115 H	-3.72800	-0.49500	0.28100 H_	1 0	0.00000
HETATM	116 H	-4.79900	1.40900	1.06400 H_	1 0	0.00000
HETATM	117 H	-1.98100	1.95700	3.74300 H_	1 0	0.00000
HETATM	118 H	-8.36800	0.53700	3.92900 H_	1 0	0.00000
HETATM	119 H	-8.53000	-0.82900	5.80800 H_	1 0	0.00000
HETATM	120 H	-6.89800	-0.71200	7.47600 H_	1 0	0.00000
HETATM	121 H	-5.11900	0.75000	7.25400 H_	1 0	0.00000
HETATM	122 H	-3.78600	2.30400	6.98900 H_	1 0	0.00000
HETATM	123 H	-1.78400	3.06800	7.77800 H_	1 0	0.00000
HETATM	124 H	0.09000	4.43100	7.66700 H_	1 0	0.00000
HETATM	125 H	0.38100	5.84200	5.86100 H_	1 0	0.00000
HETATM	126 H	-8.23100	2.09200	2.63700 H_	1 0	0.00000
HETATM	127 H	-7.73300	5.85600	-1.46100 H_	1 0	0.00000

HETATM	128 H	-9.48400	4.39300	-0.99000 H_	1 0 0.00000
HETATM	129 H	-9.30600	2.93800	0.80500 H_	1 0 0.00000
HETATM	130 H	-3.06400	6.95800	3.52100 H_	1 0 0.00000
HETATM	131 H	-2.05800	8.00600	2.84900 H_	1 0 0.00000
HETATM	132 H	-2.21300	7.95200	4.44200 H_	1 0 0.00000
HETATM	133 H	-1.87700	5.17300	2.17600 H_	1 0 0.00000
HETATM	134 H	-0.32900	4.88000	2.45200 H_	1 0 0.00000
HETATM	135 H	-0.76400	6.18300	1.63100 H_	1 0 0.00000
HETATM	136 H	0.45000	7.65600	3.02900 H_	1 0 0.00000
HETATM	137 H	0.98200	6.50700	4.00800 H_	1 0 0.00000
HETATM	138 H	0.20200	7.77000	4.60700 H_	1 0 0.00000
HETATM	139 H	-5.86400	6.62200	-2.35100 H_	1 0 0.00000
HETATM	140 H	-4.98700	7.80600	-1.72600 H_	1 0 0.00000
HETATM	141 H	-6.53500	7.67200	-1.34500 H_	1 0 0.00000
HETATM	142 H	-5.84900	7.70600	1.07000 H_	1 0 0.00000
HETATM	143 H	-4.31600	7.80000	0.62500 H_	1 0 0.00000
HETATM	144 H	-4.78800	6.63900	1.61500 H_	1 0 0.00000
HETATM	145 H	-3.75800	4.99400	0.04200 H_	1 0 0.00000
HETATM	146 H	-3.35900	6.16900	-0.96900 H_	1 0 0.00000
HETATM	147 H	-4.22800	4.93100	-1.48800 H_	1 0 0.00000
HETATM	148 Zn	-0.59300	-5.74000	3.37300 Zn	1 0 0.00000
HETATM	149 O	-2.38300	-5.25100	3.96500 O_3	2 0 0.00000
HETATM	150 O	-1.16900	-6.70000	1.76500 O_3	2 0 0.00000
HETATM	151 N	0.14000	-3.94700	2.48400 N_R	2 0 0.00000
HETATM	152 N	0.13700	-5.29000	5.28100 N_2	3 0 0.00000
HETATM	153 N	1.16400	-6.84300	3.40000 N_2	3 0 0.00000
HETATM	154 C	0.48600	-1.56800	2.57400 C_R	3 0 0.00000
HETATM	155 C	1.38900	-1.66400	1.53400 C_R	3 0 0.00000
HETATM	156 C	1.66000	-2.90000	0.98500 C_R	3 0 0.00000
HETATM	157 C	1.00800	-4.01900	1.46600 C_R	3 0 0.00000
HETATM	158 C	-0.09600	-2.74700	3.01600 C_R	3 0 0.00000
HETATM	159 C	1.47100	-5.71700	5.48400 C_R	3 0 0.00000
HETATM	160 C	2.01600	-6.53700	4.48300 C_R	3 0 0.00000
HETATM	161 C	3.33600	-6.97800	4.61400 C_R	3 0 0.00000
HETATM	162 C	4.09400	-6.64900	5.72200 C_R	3 0 0.00000
HETATM	163 C	3.55000	-5.84500	6.71000 C_R	3 0 0.00000
HETATM	164 C	2.26600	-5.37700	6.58200 C_R	3 0 0.00000
HETATM	165 C	-0.53500	-4.61700	6.16400 C_3	4 0 0.00000
HETATM	166 C	-1.88100	-4.12500	6.00300 C_R	3 0 0.00000
HETATM	167 C	-2.33200	-3.26900	7.03700 C_R	3 0 0.00000
HETATM	168 C	-3.57900	-2.71600	6.97500 C_R	3 0 0.00000
HETATM	169 C	-4.39400	-3.00300	5.89200 C_R	3 0 0.00000
HETATM	170 C	-4.05400	-3.84100	4.86600 C_R	3 0 0.00000
HETATM	171 C	-2.72500	-4.43800	4.90700 C_R	3 0 0.00000
HETATM	172 C	1.46700	-7.74100	2.52100 C_3	4 0 0.00000
HETATM	173 C	0.68300	-8.16200	1.38700 C_R	3 0 0.00000
HETATM	174 C	-0.62600	-7.65000	1.08000 C_R	3 0 0.00000
HETATM	175 C	-1.34200	-8.24300	-0.02400 C_R	3 0 0.00000
HETATM	176 C	-0.73000	-9.24100	-0.73700 C_R	3 0 0.00000
HETATM	177 C	0.55300	-9.72500	-0.45700 C_R	3 0 0.00000

HETATM	178 C	1.24100	-9.19700	0.59700 C_R	3 0	0.00000
HETATM	179 C	-4.99300	-4.13800	3.69400 C_3	4 0	0.00000
HETATM	180 C	-5.32100	-5.61800	3.62100 C_3	4 0	0.00000
HETATM	181 C	-4.33000	-3.66300	2.36500 C_3	4 0	0.00000
HETATM	182 C	-6.32300	-3.34800	3.85000 C_3	4 0	0.00000
HETATM	183 C	-2.76000	-7.76200	-0.36300 C_3	4 0	0.00000
HETATM	184 C	-3.35600	-8.53800	-1.55400 C_3	4 0	0.00000
HETATM	185 C	-3.70100	-7.96500	0.84700 C_3	4 0	0.00000
HETATM	186 C	-2.75600	-6.27400	-0.72800 C_3	4 0	0.00000
HETATM	187 H	1.81900	-0.88500	1.19700 H_	1 0	0.00000
HETATM	188 H	2.29300	-2.98100	0.28100 H_	1 0	0.00000
HETATM	189 H	1.17900	-4.86100	1.06400 H_	1 0	0.00000
HETATM	190 H	-0.70400	-2.69400	3.74300 H_	1 0	0.00000
HETATM	191 H	3.71900	-7.51500	3.92900 H_	1 0	0.00000
HETATM	192 H	4.98300	-6.97300	5.80800 H_	1 0	0.00000
HETATM	193 H	4.06500	-5.61800	7.47600 H_	1 0	0.00000
HETATM	194 H	1.91000	-4.80800	7.25400 H_	1 0	0.00000
HETATM	195 H	-0.10200	-4.43100	6.98900 H_	1 0	0.00000
HETATM	196 H	-1.76500	-3.07900	7.77800 H_	1 0	0.00000
HETATM	197 H	-3.88200	-2.13800	7.66700 H_	1 0	0.00000
HETATM	198 H	-5.24900	-2.59100	5.86100 H_	1 0	0.00000
HETATM	199 H	2.30300	-8.17400	2.63700 H_	1 0	0.00000
HETATM	200 H	-1.20500	-9.62500	-1.46100 H_	1 0	0.00000
HETATM	201 H	0.93800	-10.41000	-0.99000 H_	1 0	0.00000
HETATM	202 H	2.10800	-9.52800	0.80500 H_	1 0	0.00000
HETATM	203 H	-4.49400	-6.13300	3.52100 H_	1 0	0.00000
HETATM	204 H	-5.90500	-5.78600	2.84900 H_	1 0	0.00000
HETATM	205 H	-5.78000	-5.89200	4.44200 H_	1 0	0.00000
HETATM	206 H	-3.54200	-4.21200	2.17600 H_	1 0	0.00000
HETATM	207 H	-4.06200	-2.72500	2.45200 H_	1 0	0.00000
HETATM	208 H	-4.97300	-3.75300	1.63100 H_	1 0	0.00000
HETATM	209 H	-6.85500	-3.43900	3.02900 H_	1 0	0.00000
HETATM	210 H	-6.12600	-2.40300	4.00800 H_	1 0	0.00000
HETATM	211 H	-6.83000	-3.71000	4.60700 H_	1 0	0.00000
HETATM	212 H	-2.80300	-8.38900	-2.35100 H_	1 0	0.00000
HETATM	213 H	-4.26700	-8.22100	-1.72600 H_	1 0	0.00000
HETATM	214 H	-3.37700	-9.49500	-1.34500 H_	1 0	0.00000
HETATM	215 H	-3.74900	-8.91900	1.07000 H_	1 0	0.00000
HETATM	216 H	-4.59700	-7.63800	0.62500 H_	1 0	0.00000
HETATM	217 H	-3.35500	-7.46600	1.61500 H_	1 0	0.00000
HETATM	218 H	-2.44600	-5.75100	0.04200 H_	1 0	0.00000
HETATM	219 H	-3.66300	-5.99400	-0.96900 H_	1 0	0.00000
HETATM	220 H	-2.15600	-6.12700	-1.48800 H_	1 0	0.00000

3b-out:

HETATM	1 Zn	6.05100	7.34300	8.34700 Zn	1 0	0.00000
HETATM	2 P	10.43200	6.02300	11.98800 P_3	1 0	0.00000
HETATM	3 O	5.47800	5.72200	9.31100 O_3	2 0	0.00000
HETATM	4 O	4.58700	8.49300	8.95800 O_3	2 0	0.00000
HETATM	5 N	7.53400	7.89700	9.74900 N_R	2 0	0.00000

HETATM	6 N	7.01600	6.16100	6.94700	N_2	3 0	0.00000
HETATM	7 N	6.37700	8.73600	6.80300	N_2	3 0	0.00000
HETATM	8 C	9.32800	7.25700	11.21400	C_R	3 0	0.00000
HETATM	9 C	8.42300	6.99600	10.20000	C_R	3 0	0.00000
HETATM	10 C	7.53200	9.10700	10.31300	C_R	3 0	0.00000
HETATM	11 C	8.41100	9.46600	11.32200	C_R	3 0	0.00000
HETATM	12 C	9.30800	8.53200	11.77200	C_R	3 0	0.00000
HETATM	13 C	7.49900	6.87300	5.81400	C_R	3 0	0.00000
HETATM	14 C	8.22600	6.30100	4.77400	C_R	3 0	0.00000
HETATM	15 C	8.61900	7.06100	3.69100	C_R	3 0	0.00000
HETATM	16 C	8.31800	8.40400	3.63500	C_R	3 0	0.00000
HETATM	17 C	7.60900	8.99100	4.64600	C_R	3 0	0.00000
HETATM	18 C	7.18000	8.24500	5.74400	C_R	3 0	0.00000
HETATM	19 C	7.12100	4.87100	7.02900	C_3	4 0	0.00000
HETATM	20 C	6.58000	4.01700	8.05600	C_R	3 0	0.00000
HETATM	21 C	5.74400	4.46700	9.11600	C_R	3 0	0.00000
HETATM	22 C	5.14700	3.48000	9.98300	C_R	3 0	0.00000
HETATM	23 C	5.44400	2.15700	9.75200	C_R	3 0	0.00000
HETATM	24 C	6.29400	1.71500	8.73400	C_R	3 0	0.00000
HETATM	25 C	6.84700	2.64000	7.90300	C_R	3 0	0.00000
HETATM	26 C	5.96600	9.95400	6.83300	C_3	4 0	0.00000
HETATM	27 C	5.08600	10.52900	7.80600	C_R	3 0	0.00000
HETATM	28 C	4.86700	11.93100	7.69100	C_R	3 0	0.00000
HETATM	29 C	4.01300	12.55300	8.54900	C_R	3 0	0.00000
HETATM	30 C	3.33400	11.81000	9.52100	C_R	3 0	0.00000
HETATM	31 C	3.50100	10.45100	9.69200	C_R	3 0	0.00000
HETATM	32 C	4.40900	9.77200	8.81200	C_R	3 0	0.00000
HETATM	33 C	4.21900	3.91700	11.12500	C_3	4 0	0.00000
HETATM	34 C	5.00300	4.80600	12.10700	C_3	4 0	0.00000
HETATM	35 C	3.67000	2.71000	11.89500	C_3	4 0	0.00000
HETATM	36 C	3.00800	4.68200	10.56100	C_3	4 0	0.00000
HETATM	37 C	2.79100	9.66200	10.81000	C_3	4 0	0.00000
HETATM	38 C	1.83700	10.55400	11.60100	C_3	4 0	0.00000
HETATM	39 C	3.83000	9.09400	11.78100	C_3	4 0	0.00000
HETATM	40 C	1.94900	8.53600	10.21500	C_3	4 0	0.00000
HETATM	41 H	8.43000	6.13400	9.80100	H_	1 0	0.00000
HETATM	42 H	6.89900	9.74800	10.01300	H_	1 0	0.00000
HETATM	43 H	8.39600	10.33900	11.69100	H_	1 0	0.00000
HETATM	44 H	9.91500	8.75600	12.46900	H_	1 0	0.00000
HETATM	45 H	8.45200	5.37700	4.80800	H_	1 0	0.00000
HETATM	46 H	9.10300	6.65700	2.98100	H_	1 0	0.00000
HETATM	47 H	8.60400	8.92300	2.89100	H_	1 0	0.00000
HETATM	48 H	7.40400	9.91800	4.60100	H_	1 0	0.00000
HETATM	49 H	7.60900	4.44100	6.33300	H_	1 0	0.00000
HETATM	50 H	5.04700	1.50700	10.32000	H_	1 0	0.00000
HETATM	51 H	6.48200	0.79000	8.62500	H_	1 0	0.00000
HETATM	52 H	7.42100	2.35300	7.20600	H_	1 0	0.00000
HETATM	53 H	6.27500	10.52900	6.14200	H_	1 0	0.00000
HETATM	54 H	5.31400	12.43200	7.02100	H_	1 0	0.00000
HETATM	55 H	3.88000	13.49200	8.48800	H_	1 0	0.00000

HETATM	56 H	2.72500	12.26500	10.09200 H_	1 0 0.00000
HETATM	57 H	5.75800	4.30200	12.47500 H_	1 0 0.00000
HETATM	58 H	4.41100	5.08800	12.83500 H_	1 0 0.00000
HETATM	59 H	5.33700	5.59800	11.63800 H_	1 0 0.00000
HETATM	60 H	4.41600	2.20300	12.27900 H_	1 0 0.00000
HETATM	61 H	3.16500	2.13600	11.28300 H_	1 0 0.00000
HETATM	62 H	3.08100	3.02300	12.61200 H_	1 0 0.00000
HETATM	63 H	2.43500	4.97600	11.29900 H_	1 0 0.00000
HETATM	64 H	2.49700	4.09400	9.96500 H_	1 0 0.00000
HETATM	65 H	3.32000	5.46400	10.06000 H_	1 0 0.00000
HETATM	66 H	1.17400	10.94400	10.99200 H_	1 0 0.00000
HETATM	67 H	2.34500	11.27200	12.03500 H_	1 0 0.00000
HETATM	68 H	1.38000	10.01900	12.28400 H_	1 0 0.00000
HETATM	69 H	3.37400	8.59700	12.49100 H_	1 0 0.00000
HETATM	70 H	4.34400	9.83000	12.17300 H_	1 0 0.00000
HETATM	71 H	4.43500	8.49400	11.29900 H_	1 0 0.00000
HETATM	72 H	1.26600	8.91500	9.62100 H_	1 0 0.00000
HETATM	73 H	1.51500	8.03700	10.93900 H_	1 0 0.00000
HETATM	74 H	2.52700	7.93200	9.70000 H_	1 0 0.00000
HETATM	75 Zn	11.47900	1.56900	8.34700 Zn	1 0 0.00000
HETATM	76 O	13.17000	1.88300	9.31100 O_3	2 0 0.00000
HETATM	77 O	11.21600	-0.27500	8.95800 O_3	2 0 0.00000
HETATM	78 N	10.25800	2.57700	9.74900 N_R	2 0 0.00000
HETATM	79 N	12.02000	2.99600	6.94700 N_2	3 0 0.00000
HETATM	80 N	10.11000	1.15500	6.80300 N_2	3 0 0.00000
HETATM	81 C	9.91600	4.45000	11.21400 C_R	3 0 0.00000
HETATM	82 C	10.59400	3.79600	10.20000 C_R	3 0 0.00000
HETATM	83 C	9.21200	1.97000	10.31300 C_R	3 0 0.00000
HETATM	84 C	8.46100	2.55100	11.32200 C_R	3 0 0.00000
HETATM	85 C	8.82100	3.79500	11.77200 C_R	3 0 0.00000
HETATM	86 C	11.16200	3.05700	5.81400 C_R	3 0 0.00000
HETATM	87 C	11.29500	3.97300	4.77400 C_R	3 0 0.00000
HETATM	88 C	10.44000	3.93400	3.69100 C_R	3 0 0.00000
HETATM	89 C	9.42800	3.00100	3.63500 C_R	3 0 0.00000
HETATM	90 C	9.27300	2.09400	4.64600 C_R	3 0 0.00000
HETATM	91 C	10.13400	2.09600	5.74400 C_R	3 0 0.00000
HETATM	92 C	13.08500	3.73100	7.02900 C_3	4 0 0.00000
HETATM	93 C	14.09600	3.69000	8.05600 C_R	3 0 0.00000
HETATM	94 C	14.12400	2.74100	9.11600 C_R	3 0 0.00000
HETATM	95 C	15.27700	2.71800	9.98300 C_R	3 0 0.00000
HETATM	96 C	16.27400	3.63600	9.75200 C_R	3 0 0.00000
HETATM	97 C	16.23300	4.59300	8.73400 C_R	3 0 0.00000
HETATM	98 C	15.15500	4.60900	7.90300 C_R	3 0 0.00000
HETATM	99 C	9.26100	0.19000	6.83300 C_3	4 0 0.00000
HETATM	100 C	9.20300	-0.86000	7.80600 C_R	3 0 0.00000
HETATM	101 C	8.09900	-1.75100	7.69100 C_R	3 0 0.00000
HETATM	102 C	7.98700	-2.80100	8.54900 C_R	3 0 0.00000
HETATM	103 C	8.97000	-3.01800	9.52100 C_R	3 0 0.00000
HETATM	104 C	10.06300	-2.19400	9.69200 C_R	3 0 0.00000
HETATM	105 C	10.19700	-1.06800	8.81200 C_R	3 0 0.00000

HETATM	106 C	15.36200	1.69500	11.12500 C_3	4 0 0.00000
HETATM	107 C	14.20000	1.93000	12.10700 C_3	4 0 0.00000
HETATM	108 C	16.68200	1.82300	11.89500 C_3	4 0 0.00000
HETATM	109 C	15.30600	0.26400	10.56100 C_3	4 0 0.00000
HETATM	110 C	11.10200	-2.41400	10.81000 C_3	4 0 0.00000
HETATM	111 C	10.80600	-3.68600	11.60100 C_3	4 0 0.00000
HETATM	112 C	11.07400	-1.23100	11.78100 C_3	4 0 0.00000
HETATM	113 C	12.49800	-2.58000	10.21500 C_3	4 0 0.00000
HETATM	114 H	11.33700	4.23400	9.80100 H_	1 0 0.00000
HETATM	115 H	8.97300	1.10000	10.01300 H_	1 0 0.00000
HETATM	116 H	7.71300	2.10100	11.69100 H_	1 0 0.00000
HETATM	117 H	8.32400	4.20800	12.46900 H_	1 0 0.00000
HETATM	118 H	11.98100	4.63100	4.80800 H_	1 0 0.00000
HETATM	119 H	10.54800	4.55500	2.98100 H_	1 0 0.00000
HETATM	120 H	8.83500	2.99000	2.89100 H_	1 0 0.00000
HETATM	121 H	8.57300	1.45300	4.60100 H_	1 0 0.00000
HETATM	122 H	13.21300	4.36900	6.33300 H_	1 0 0.00000
HETATM	123 H	17.03600	3.61700	10.32000 H_	1 0 0.00000
HETATM	124 H	16.94000	5.21800	8.62500 H_	1 0 0.00000
HETATM	125 H	15.11600	5.25100	7.20600 H_	1 0 0.00000
HETATM	126 H	8.60900	0.17000	6.14200 H_	1 0 0.00000
HETATM	127 H	7.44100	-1.61400	7.02100 H_	1 0 0.00000
HETATM	128 H	7.24000	-3.38600	8.48800 H_	1 0 0.00000
HETATM	129 H	8.88000	-3.77300	10.09200 H_	1 0 0.00000
HETATM	130 H	14.26000	2.83500	12.47500 H_	1 0 0.00000
HETATM	131 H	14.25200	1.27600	12.83500 H_	1 0 0.00000
HETATM	132 H	13.34800	1.82300	11.63800 H_	1 0 0.00000
HETATM	133 H	16.74900	2.72300	12.27900 H_	1 0 0.00000
HETATM	134 H	17.43200	1.67300	11.28300 H_	1 0 0.00000
HETATM	135 H	16.70600	1.15600	12.61200 H_	1 0 0.00000
HETATM	136 H	15.33700	-0.37900	11.29900 H_	1 0 0.00000
HETATM	137 H	16.07000	0.11600	9.96500 H_	1 0 0.00000
HETATM	138 H	14.47300	0.14300	10.06000 H_	1 0 0.00000
HETATM	139 H	10.79900	-4.45600	10.99200 H_	1 0 0.00000
HETATM	140 H	9.93000	-3.60500	12.03500 H_	1 0 0.00000
HETATM	141 H	11.49700	-3.81400	12.28400 H_	1 0 0.00000
HETATM	142 H	11.73200	-1.37700	12.49100 H_	1 0 0.00000
HETATM	143 H	10.18000	-1.15300	12.17300 H_	1 0 0.00000
HETATM	144 H	11.29100	-0.40700	11.29900 H_	1 0 0.00000
HETATM	145 H	12.51000	-3.36100	9.62100 H_	1 0 0.00000
HETATM	146 H	13.14700	-2.70700	10.93900 H_	1 0 0.00000
HETATM	147 H	12.73100	-1.77800	9.70000 H_	1 0 0.00000
HETATM	148 Zn	13.76600	9.15700	8.34700 Zn	1 0 0.00000
HETATM	149 O	12.64900	10.46400	9.31100 O_3	2 0 0.00000
HETATM	150 O	15.49400	9.85000	8.95800 O_3	2 0 0.00000
HETATM	151 N	13.50300	7.59600	9.74900 N_R	2 0 0.00000
HETATM	152 N	12.26000	8.91200	6.94700 N_2	3 0 0.00000
HETATM	153 N	14.80900	8.17900	6.80300 N_2	3 0 0.00000
HETATM	154 C	12.05200	6.36200	11.21400 C_R	3 0 0.00000
HETATM	155 C	12.28000	7.27600	10.20000 C_R	3 0 0.00000

HETATM	156 C	14.55300	6.99300	10.31300 C_R	3 0 0.00000
HETATM	157 C	14.42500	6.05100	11.32200 C_R	3 0 0.00000
HETATM	158 C	13.16800	5.74200	11.77200 C_R	3 0 0.00000
HETATM	159 C	12.63500	8.13800	5.81400 C_R	3 0 0.00000
HETATM	160 C	11.77600	7.79500	4.77400 C_R	3 0 0.00000
HETATM	161 C	12.23800	7.07400	3.69100 C_R	3 0 0.00000
HETATM	162 C	13.55100	6.66400	3.63500 C_R	3 0 0.00000
HETATM	163 C	14.41400	6.98400	4.64600 C_R	3 0 0.00000
HETATM	164 C	13.98200	7.72800	5.74400 C_R	3 0 0.00000
HETATM	165 C	11.09000	9.46600	7.02900 C_3	4 0 0.00000
HETATM	166 C	10.62100	10.36300	8.05600 C_R	3 0 0.00000
HETATM	167 C	11.42800	10.86100	9.11600 C_R	3 0 0.00000
HETATM	168 C	10.87200	11.87100	9.98300 C_R	3 0 0.00000
HETATM	169 C	9.57900	12.27600	9.75200 C_R	3 0 0.00000
HETATM	170 C	8.77000	11.76100	8.73400 C_R	3 0 0.00000
HETATM	171 C	9.29500	10.82000	7.90300 C_R	3 0 0.00000
HETATM	172 C	16.07000	7.92500	6.83300 C_3	4 0 0.00000
HETATM	173 C	17.00800	8.40000	7.80600 C_R	3 0 0.00000
HETATM	174 C	18.33100	7.88900	7.69100 C_R	3 0 0.00000
HETATM	175 C	19.29600	8.31700	8.54900 C_R	3 0 0.00000
HETATM	176 C	18.99300	9.27700	9.52100 C_R	3 0 0.00000
HETATM	177 C	17.73300	9.81200	9.69200 C_R	3 0 0.00000
HETATM	178 C	16.69000	9.36500	8.81200 C_R	3 0 0.00000
HETATM	179 C	11.71500	12.45700	11.12500 C_3	4 0 0.00000
HETATM	180 C	12.09300	11.33300	12.10700 C_3	4 0 0.00000
HETATM	181 C	10.94400	13.53600	11.89500 C_3	4 0 0.00000
HETATM	182 C	12.98300	13.12400	10.56100 C_3	4 0 0.00000
HETATM	183 C	17.40400	10.82200	10.81000 C_3	4 0 0.00000
HETATM	184 C	18.65400	11.20100	11.60100 C_3	4 0 0.00000
HETATM	185 C	16.39300	10.20500	11.78100 C_3	4 0 0.00000
HETATM	186 C	16.85000	12.11400	10.21500 C_3	4 0 0.00000
HETATM	187 H	11.53000	7.70100	9.80100 H_	1 0 0.00000
HETATM	188 H	15.42500	7.22000	10.01300 H_	1 0 0.00000
HETATM	189 H	15.18800	5.62900	11.69100 H_	1 0 0.00000
HETATM	190 H	13.05800	5.10500	12.46900 H_	1 0 0.00000
HETATM	191 H	10.86300	8.06100	4.80800 H_	1 0 0.00000
HETATM	192 H	11.64500	6.85700	2.98100 H_	1 0 0.00000
HETATM	193 H	13.85700	6.15600	2.89100 H_	1 0 0.00000
HETATM	194 H	15.32000	6.69800	4.60100 H_	1 0 0.00000
HETATM	195 H	10.47400	9.25900	6.33300 H_	1 0 0.00000
HETATM	196 H	9.21400	12.94500	10.32000 H_	1 0 0.00000
HETATM	197 H	7.87500	12.06100	8.62500 H_	1 0 0.00000
HETATM	198 H	8.75900	10.46600	7.20600 H_	1 0 0.00000
HETATM	199 H	16.41300	7.37000	6.14200 H_	1 0 0.00000
HETATM	200 H	18.54100	7.25100	7.02100 H_	1 0 0.00000
HETATM	201 H	20.17700	7.96300	8.48800 H_	1 0 0.00000
HETATM	202 H	19.69200	9.57700	10.09200 H_	1 0 0.00000
HETATM	203 H	11.27900	10.93200	12.47500 H_	1 0 0.00000
HETATM	204 H	12.63300	11.70500	12.83500 H_	1 0 0.00000
HETATM	205 H	12.61100	10.64800	11.63800 H_	1 0 0.00000

HETATM	206 H	10.13200	13.14300	12.27900	H_	1 0	0.00000
HETATM	207 H	10.69900	14.26000	11.28300	H_	1 0	0.00000
HETATM	208 H	11.51000	13.89000	12.61200	H_	1 0	0.00000
HETATM	209 H	13.52400	13.47200	11.29900	H_	1 0	0.00000
HETATM	210 H	12.72900	13.85900	9.96500	H_	1 0	0.00000
HETATM	211 H	13.50400	12.46200	10.06000	H_	1 0	0.00000
HETATM	212 H	19.32400	11.58000	10.99200	H_	1 0	0.00000
HETATM	213 H	19.02100	10.40200	12.03500	H_	1 0	0.00000
HETATM	214 H	18.41900	11.86400	12.28400	H_	1 0	0.00000
HETATM	215 H	16.19100	10.84900	12.49100	H_	1 0	0.00000
HETATM	216 H	16.77300	9.39200	12.17300	H_	1 0	0.00000
HETATM	217 H	15.57100	9.98100	11.29900	H_	1 0	0.00000
HETATM	218 H	17.52000	12.51500	9.62100	H_	1 0	0.00000
HETATM	219 H	16.63500	12.73900	10.93900	H_	1 0	0.00000
HETATM	220 H	16.03800	11.91500	9.70000	H_	1 0	0.00000

3g-in:

HETATM	1 Ru	45.44168	42.34286	40.23485	Ru	0 0	0.00000
HETATM	2 P	40.04673	40.05181	40.35298	P	0 0	0.00000
HETATM	3 O	45.43582	40.50899	40.49448	O	0 0	0.00000
HETATM	4 O	45.98673	42.31303	38.43221	O	0 0	0.00000
HETATM	5 N	43.45075	42.11299	39.45126	N	0 0	0.00000
HETATM	6 N	44.42106	42.68701	42.11695	N	0 0	0.00000
HETATM	7 N	45.28006	44.50977	40.09198	N	0 0	0.00000
HETATM	8 C	41.26329	41.12302	39.47363	C	0 0	0.00000
HETATM	9 C	40.81728	41.95423	38.40030	C	0 0	0.00000
HETATM	10 C	41.77484	42.84721	37.85917	C	0 0	0.00000
HETATM	11 C	43.06226	42.88100	38.42172	C	0 0	0.00000
HETATM	12 C	42.57898	41.24703	39.95587	C	0 0	0.00000
HETATM	13 C	44.13179	44.09842	42.26829	C	0 0	0.00000
HETATM	14 C	44.55485	45.02440	41.22957	C	0 0	0.00000
HETATM	15 C	44.28400	46.41634	41.40752	C	0 0	0.00000
HETATM	16 C	43.62822	46.91907	42.55292	C	0 0	0.00000
HETATM	17 C	43.20289	46.01128	43.56636	C	0 0	0.00000
HETATM	18 C	43.45362	44.63022	43.40692	C	0 0	0.00000
HETATM	19 C	44.12503	41.79252	42.96440	C	0 0	0.00000
HETATM	20 C	44.40484	40.38388	42.79321	C	0 0	0.00000
HETATM	21 C	43.97566	39.56245	43.88374	C	0 0	0.00000
HETATM	22 C	44.15916	38.17288	43.81893	C	0 0	0.00000
HETATM	23 C	44.79928	37.59158	42.69910	C	0 0	0.00000
HETATM	24 C	45.25330	38.38138	41.61261	C	0 0	0.00000
HETATM	25 C	45.04156	39.81281	41.61658	C	0 0	0.00000
HETATM	26 C	45.81929	45.21873	39.18923	C	0 0	0.00000
HETATM	27 C	46.62849	44.68713	38.11603	C	0 0	0.00000
HETATM	28 C	46.75952	43.26280	37.81270	C	0 0	0.00000
HETATM	29 C	47.71985	42.90965	36.78814	C	0 0	0.00000
HETATM	30 C	48.40152	43.91766	36.06173	C	0 0	0.00000
HETATM	31 C	48.20902	45.29258	36.33968	C	0 0	0.00000
HETATM	32 C	47.34408	45.68261	37.37375	C	0 0	0.00000
HETATM	33 C	45.97087	37.71803	40.48356	C	0 0	0.00000

HETATM	34 C	47.41223	38.25681	40.43522	C	0 0	0.00000
HETATM	35 C	45.29071	38.01092	39.13577	C	0 0	0.00000
HETATM	36 C	46.02106	36.19131	40.65049	C	0 0	0.00000
HETATM	37 C	48.03394	41.48713	36.46948	C	0 0	0.00000
HETATM	38 C	49.03620	41.35375	35.31162	C	0 0	0.00000
HETATM	39 C	48.64197	40.82390	37.71896	C	0 0	0.00000
HETATM	40 C	46.76366	40.71542	36.07228	C	0 0	0.00000
HETATM	41 H	39.78077	41.90328	38.00859	H	0 0	0.00000
HETATM	42 H	41.50758	43.51954	37.01247	H	0 0	0.00000
HETATM	43 H	43.85727	43.57521	38.02355	H	0 0	0.00000
HETATM	44 H	42.96449	40.61543	40.79996	H	0 0	0.00000
HETATM	45 H	44.59916	47.14803	40.63508	H	0 0	0.00000
HETATM	46 H	43.44717	48.00940	42.66265	H	0 0	0.00000
HETATM	47 H	42.68173	46.38597	44.47238	H	0 0	0.00000
HETATM	48 H	43.10489	43.95284	44.21408	H	0 0	0.00000
HETATM	49 H	43.61517	42.15622	43.89285	H	0 0	0.00000
HETATM	50 H	43.49567	40.01440	44.77430	H	0 0	0.00000
HETATM	51 H	43.81115	37.52683	44.65519	H	0 0	0.00000
HETATM	52 H	44.94599	36.49426	42.68956	H	0 0	0.00000
HETATM	53 H	45.69665	46.32430	39.30707	H	0 0	0.00000
HETATM	54 H	49.11024	43.64282	35.25594	H	0 0	0.00000
HETATM	55 H	48.75676	46.06175	35.75190	H	0 0	0.00000
HETATM	56 H	47.22707	46.75691	37.61483	H	0 0	0.00000
HETATM	57 H	47.41329	39.37893	40.35508	H	0 0	0.00000
HETATM	58 H	47.98649	37.84643	39.56155	H	0 0	0.00000
HETATM	59 H	47.97963	37.98883	41.36729	H	0 0	0.00000
HETATM	60 H	45.39728	39.09270	38.84268	H	0 0	0.00000
HETATM	61 H	44.19126	37.78296	39.18017	H	0 0	0.00000
HETATM	62 H	45.73348	37.39647	38.30635	H	0 0	0.00000
HETATM	63 H	46.48628	35.69266	39.75817	H	0 0	0.00000
HETATM	64 H	44.98957	35.75989	40.77402	H	0 0	0.00000
HETATM	65 H	46.62491	35.89478	41.55112	H	0 0	0.00000
HETATM	66 H	48.63288	41.81097	34.36726	H	0 0	0.00000
HETATM	67 H	49.26846	40.27841	35.08761	H	0 0	0.00000
HETATM	68 H	50.01012	41.86232	35.54839	H	0 0	0.00000
HETATM	69 H	49.61491	41.30875	38.00263	H	0 0	0.00000
HETATM	70 H	48.84610	39.73220	37.55302	H	0 0	0.00000
HETATM	71 H	47.94621	40.92138	38.60070	H	0 0	0.00000
HETATM	72 H	46.02784	40.67340	36.92143	H	0 0	0.00000
HETATM	73 H	46.99921	39.65857	35.77484	H	0 0	0.00000
HETATM	74 H	46.24662	41.20638	35.20458	H	0 0	0.00000
HETATM	75 Ru	35.23697	43.55128	40.23544	Ru	0 0	0.00000
HETATM	76 O	36.83927	44.45296	40.49458	O	0 0	0.00000
HETATM	77 O	35.00013	44.03179	38.43773	O	0 0	0.00000
HETATM	78 N	36.41852	41.94445	39.44475	N	0 0	0.00000
HETATM	79 N	35.46001	42.48818	42.11756	N	0 0	0.00000
HETATM	80 N	33.45322	42.32129	40.09335	N	0 0	0.00000
HETATM	81 C	38.38791	40.55971	39.45929	C	0 0	0.00000
HETATM	82 C	37.90324	39.74651	38.40532	C	0 0	0.00000
HETATM	83 C	36.63143	40.12121	37.85601	C	0 0	0.00000

HETATM	84 C	35.95450	41.21325	38.40763	C	0 0	0.00000
HETATM	85 C	37.63876	41.61554	39.95356	C	0 0	0.00000
HETATM	86 C	34.38374	41.53050	42.26822	C	0 0	0.00000
HETATM	87 C	33.37083	41.43377	41.23054	C	0 0	0.00000
HETATM	88 C	32.30147	40.50240	41.40750	C	0 0	0.00000
HETATM	89 C	32.19374	39.68261	42.55295	C	0 0	0.00000
HETATM	90 C	33.19255	39.76840	43.56620	C	0 0	0.00000
HETATM	91 C	34.26324	40.67667	43.40644	C	0 0	0.00000
HETATM	92 C	36.38409	42.67658	42.96306	C	0 0	0.00000
HETATM	93 C	37.46412	43.62365	42.79331	C	0 0	0.00000
HETATM	94 C	38.39036	43.66201	43.88352	C	0 0	0.00000
HETATM	95 C	39.50269	44.51597	43.81853	C	0 0	0.00000
HETATM	96 C	39.68596	45.36087	42.69886	C	0 0	0.00000
HETATM	97 C	38.77493	45.35931	41.61270	C	0 0	0.00000
HETATM	98 C	37.64015	44.46067	41.61630	C	0 0	0.00000
HETATM	99 C	32.57100	42.43100	39.18943	C	0 0	0.00000
HETATM	100 C	32.62480	43.39730	38.11646	C	0 0	0.00000
HETATM	101 C	33.79280	44.22417	37.81407	C	0 0	0.00000
HETATM	102 C	33.62022	45.23099	36.78860	C	0 0	0.00000
HETATM	103 C	32.40623	45.31724	36.06146	C	0 0	0.00000
HETATM	104 C	31.31199	44.46312	36.33967	C	0 0	0.00000
HETATM	105 C	31.40594	43.51917	37.37330	C	0 0	0.00000
HETATM	106 C	38.99073	46.31196	40.48360	C	0 0	0.00000
HETATM	107 C	37.80344	47.29093	40.43506	C	0 0	0.00000
HETATM	108 C	39.07715	45.57655	39.13568	C	0 0	0.00000
HETATM	109 C	40.28780	47.11898	40.65041	C	0 0	0.00000
HETATM	110 C	34.69509	46.21396	36.46962	C	0 0	0.00000
HETATM	111 C	34.30973	47.14852	35.31191	C	0 0	0.00000
HETATM	112 C	34.96555	47.07212	37.71882	C	0 0	0.00000
HETATM	113 C	35.99846	45.50002	36.07243	C	0 0	0.00000
HETATM	114 H	38.47298	38.87014	38.02387	H	0 0	0.00000
HETATM	115 H	36.18733	39.54775	37.00998	H	0 0	0.00000
HETATM	116 H	34.95521	41.54904	38.00453	H	0 0	0.00000
HETATM	117 H	38.00098	42.26117	40.80047	H	0 0	0.00000
HETATM	118 H	31.50999	40.40900	40.63534	H	0 0	0.00000
HETATM	119 H	31.34011	38.98051	42.66279	H	0 0	0.00000
HETATM	120 H	33.12887	39.12956	44.47239	H	0 0	0.00000
HETATM	121 H	35.02404	40.71269	44.21397	H	0 0	0.00000
HETATM	122 H	36.32534	42.05111	43.89006	H	0 0	0.00000
HETATM	123 H	38.23950	43.02035	44.77429	H	0 0	0.00000
HETATM	124 H	40.23631	44.53728	44.65504	H	0 0	0.00000
HETATM	125 H	40.56336	46.03631	42.68937	H	0 0	0.00000
HETATM	126 H	31.67574	41.76966	39.30614	H	0 0	0.00000
HETATM	127 H	32.28997	46.06810	35.25550	H	0 0	0.00000
HETATM	128 H	30.37179	44.55303	35.75180	H	0 0	0.00000
HETATM	129 H	30.53435	42.88085	37.61477	H	0 0	0.00000
HETATM	130 H	36.83117	46.73078	40.35493	H	0 0	0.00000
HETATM	131 H	37.87166	47.99351	39.56141	H	0 0	0.00000
HETATM	132 H	37.75176	47.91630	41.36709	H	0 0	0.00000
HETATM	133 H	38.08701	45.12826	38.84229	H	0 0	0.00000

HETATM	134	H	39.82394	44.73816	39.18029	H	0 0	0.00000
HETATM	135	H	39.38840	46.26703	38.30627	H	0 0	0.00000
HETATM	136	H	40.48706	47.77135	39.75814	H	0 0	0.00000
HETATM	137	H	41.17718	46.44147	40.77394	H	0 0	0.00000
HETATM	138	H	40.24265	47.79009	41.55111	H	0 0	0.00000
HETATM	139	H	34.11547	46.57080	34.36731	H	0 0	0.00000
HETATM	140	H	35.12456	47.88765	35.08760	H	0 0	0.00000
HETATM	141	H	33.38215	47.73772	35.54838	H	0 0	0.00000
HETATM	142	H	34.05913	47.67227	38.00269	H	0 0	0.00000
HETATM	143	H	35.80868	47.79527	37.55294	H	0 0	0.00000
HETATM	144	H	35.22940	46.42084	38.60077	H	0 0	0.00000
HETATM	145	H	36.40297	44.88364	36.92138	H	0 0	0.00000
HETATM	146	H	36.79621	46.23236	35.77494	H	0 0	0.00000
HETATM	147	H	35.83212	44.80690	35.20449	H	0 0	0.00000
HETATM	148	Ru	39.30714	34.10232	40.23422	Ru	0 0	0.00000
HETATM	149	O	37.72415	35.03626	40.49407	O	0 0	0.00000
HETATM	150	O	39.00800	33.65406	38.43860	O	0 0	0.00000
HETATM	151	N	40.10951	35.92763	39.44089	N	0 0	0.00000
HETATM	152	N	40.11479	34.82439	42.11673	N	0 0	0.00000
HETATM	153	N	41.26284	33.16920	40.09325	N	0 0	0.00000
HETATM	154	C	40.36162	38.32678	39.47618	C	0 0	0.00000
HETATM	155	C	41.28302	38.30513	38.40495	C	0 0	0.00000
HETATM	156	C	41.58233	37.01453	37.85156	C	0 0	0.00000
HETATM	157	C	40.97435	35.88429	38.40447	C	0 0	0.00000
HETATM	158	C	39.79811	37.15458	39.95181	C	0 0	0.00000
HETATM	159	C	41.48217	34.37079	42.26857	C	0 0	0.00000
HETATM	160	C	42.07273	33.54165	41.23141	C	0 0	0.00000
HETATM	161	C	43.41451	33.08159	41.40773	C	0 0	0.00000
HETATM	162	C	44.17786	33.39840	42.55305	C	0 0	0.00000
HETATM	163	C	43.60431	34.22064	43.56612	C	0 0	0.00000
HETATM	164	C	42.28229	34.69375	43.40604	C	0 0	0.00000
HETATM	165	C	39.49028	35.52999	42.96288	C	0 0	0.00000
HETATM	166	C	38.12975	35.99179	42.79269	C	0 0	0.00000
HETATM	167	C	37.63351	36.77527	43.88365	C	0 0	0.00000
HETATM	168	C	36.33840	37.31118	43.81855	C	0 0	0.00000
HETATM	169	C	35.51451	37.04739	42.69862	C	0 0	0.00000
HETATM	170	C	35.97155	36.25908	41.61262	C	0 0	0.00000
HETATM	171	C	37.31710	35.72550	41.61491	C	0 0	0.00000
HETATM	172	C	41.60843	32.35027	39.18879	C	0 0	0.00000
HETATM	173	C	40.74447	31.91404	38.11624	C	0 0	0.00000
HETATM	174	C	39.44546	32.51127	37.81455	C	0 0	0.00000
HETATM	175	C	38.65973	31.85869	36.78835	C	0 0	0.00000
HETATM	176	C	39.19238	30.76448	36.06135	C	0 0	0.00000
HETATM	177	C	40.47886	30.24411	36.33925	C	0 0	0.00000
HETATM	178	C	41.24892	30.79816	37.37334	C	0 0	0.00000
HETATM	179	C	35.03840	35.96994	40.48374	C	0 0	0.00000
HETATM	180	C	34.78414	34.45229	40.43518	C	0 0	0.00000
HETATM	181	C	35.63215	36.41238	39.13586	C	0 0	0.00000
HETATM	182	C	33.69106	36.68976	40.65045	C	0 0	0.00000
HETATM	183	C	37.27100	32.29885	36.46971	C	0 0	0.00000

HETATM	184 C	36.65423	31.49797	35.31179	C	0 0	0.00000
HETATM	185 C	36.39260	32.10400	37.71898	C	0 0	0.00000
HETATM	186 C	37.23782	33.78469	36.07260	C	0 0	0.00000
HETATM	187 H	41.74829	39.23849	38.02088	H	0 0	0.00000
HETATM	188 H	42.29631	36.91356	37.00563	H	0 0	0.00000
HETATM	189 H	41.18092	34.85015	38.00118	H	0 0	0.00000
HETATM	190 H	39.05352	37.15248	40.79186	H	0 0	0.00000
HETATM	191 H	43.89093	32.44291	40.63502	H	0 0	0.00000
HETATM	192 H	45.21244	33.01012	42.66268	H	0 0	0.00000
HETATM	193 H	44.18944	34.48491	44.47223	H	0 0	0.00000
HETATM	194 H	41.87080	35.33481	44.21365	H	0 0	0.00000
HETATM	195 H	40.06132	35.79290	43.89020	H	0 0	0.00000
HETATM	196 H	38.26489	36.96541	44.77379	H	0 0	0.00000
HETATM	197 H	35.95274	37.93628	44.65468	H	0 0	0.00000
HETATM	198 H	34.49091	37.46971	42.68886	H	0 0	0.00000
HETATM	199 H	42.62960	31.90610	39.30471	H	0 0	0.00000
HETATM	200 H	38.60007	30.28862	35.25508	H	0 0	0.00000
HETATM	201 H	40.87127	29.38537	35.75193	H	0 0	0.00000
HETATM	202 H	42.23759	30.36237	37.61496	H	0 0	0.00000
HETATM	203 H	35.75536	33.89032	40.35505	H	0 0	0.00000
HETATM	204 H	34.14149	34.15992	39.56165	H	0 0	0.00000
HETATM	205 H	34.26858	34.09484	41.36730	H	0 0	0.00000
HETATM	206 H	36.51565	35.77924	38.84266	H	0 0	0.00000
HETATM	207 H	35.98480	37.47832	39.18037	H	0 0	0.00000
HETATM	208 H	34.87887	36.33654	38.30618	H	0 0	0.00000
HETATM	209 H	33.02630	36.53612	39.75825	H	0 0	0.00000
HETATM	210 H	33.83311	37.79877	40.77389	H	0 0	0.00000
HETATM	211 H	33.13246	36.31534	41.55127	H	0 0	0.00000
HETATM	212 H	37.25181	31.61866	34.36737	H	0 0	0.00000
HETATM	213 H	35.60676	31.83438	35.08767	H	0 0	0.00000
HETATM	214 H	36.60770	30.40017	35.54833	H	0 0	0.00000
HETATM	215 H	36.32623	31.01893	38.00273	H	0 0	0.00000
HETATM	216 H	35.34486	32.47267	37.55298	H	0 0	0.00000
HETATM	217 H	36.82488	32.65804	38.60093	H	0 0	0.00000
HETATM	218 H	37.56943	34.44305	36.92161	H	0 0	0.00000
HETATM	219 H	36.20478	34.10935	35.77506	H	0 0	0.00000
HETATM	220 H	37.92136	33.98715	35.20479	H	0 0	0.00000
HETATM	221 C	47.29069	42.60706	41.13578	C	0 0	0.00000
HETATM	222 O	48.31711	42.74994	41.63072	O	0 0	0.00000
HETATM	223 C	34.09279	45.01244	41.13689	C	0 0	0.00000
HETATM	224 O	33.45733	45.83000	41.63484	O	0 0	0.00000
HETATM	225 C	38.61291	32.37629	41.13690	C	0 0	0.00000
HETATM	226 O	38.22269	31.41714	41.63415	O	0 0	0.00000

3g-out:

HETATM	1 Ru	35.39124	41.20560	39.49541	Ru	0 0	0.00000
HETATM	2 P	39.99574	39.99993	43.13628	P	0 0	0.00000
HETATM	3 O	35.28108	39.82878	40.70515	O	0 0	0.00000
HETATM	4 O	34.39855	42.41997	40.48836	O	0 0	0.00000
HETATM	5 N	36.98691	41.77239	40.82799	N	0 0	0.00000

HETATM	6 N	36.74477	40.02657	38.26357	N	0 0	0.00000
HETATM	7 N	36.02465	42.79787	38.14419	N	0 0	0.00000
HETATM	8 C	38.83348	41.20156	42.25175	C	0 0	0.00000
HETATM	9 C	37.88700	40.87667	41.28245	C	0 0	0.00000
HETATM	10 C	37.00346	43.01069	41.37683	C	0 0	0.00000
HETATM	11 C	37.90816	43.42656	42.36001	C	0 0	0.00000
HETATM	12 C	38.87497	42.49415	42.84074	C	0 0	0.00000
HETATM	13 C	37.26276	40.84070	37.19131	C	0 0	0.00000
HETATM	14 C	37.99443	40.28438	36.09508	C	0 0	0.00000
HETATM	15 C	38.29378	41.02404	34.93100	C	0 0	0.00000
HETATM	16 C	37.97122	42.41249	34.88813	C	0 0	0.00000
HETATM	17 C	37.32597	43.00445	35.99691	C	0 0	0.00000
HETATM	18 C	36.89663	42.24614	37.12858	C	0 0	0.00000
HETATM	19 C	36.96538	38.78784	38.41221	C	0 0	0.00000
HETATM	20 C	36.29858	37.96294	39.39753	C	0 0	0.00000
HETATM	21 C	35.44183	38.48247	40.44996	C	0 0	0.00000
HETATM	22 C	34.77732	37.51063	41.28906	C	0 0	0.00000
HETATM	23 C	34.98969	36.12246	41.08715	C	0 0	0.00000
HETATM	24 C	35.83495	35.64178	40.06055	C	0 0	0.00000
HETATM	25 C	36.46699	36.55610	39.20407	C	0 0	0.00000
HETATM	26 C	35.66263	44.00981	38.18908	C	0 0	0.00000
HETATM	27 C	34.74425	44.55214	39.16752	C	0 0	0.00000
HETATM	28 C	34.42968	45.94179	39.01339	C	0 0	0.00000
HETATM	29 C	33.50559	46.54640	39.87899	C	0 0	0.00000
HETATM	30 C	32.86427	45.78208	40.88299	C	0 0	0.00000
HETATM	31 C	33.16061	44.40687	41.05657	C	0 0	0.00000
HETATM	32 C	34.13670	43.74681	40.21581	C	0 0	0.00000
HETATM	33 C	33.85078	37.91859	42.38487	C	0 0	0.00000
HETATM	34 C	34.58316	38.79948	43.41320	C	0 0	0.00000
HETATM	35 C	33.26988	36.71808	43.14871	C	0 0	0.00000
HETATM	36 C	32.68940	38.73026	41.78307	C	0 0	0.00000
HETATM	37 C	32.41959	43.65196	42.11087	C	0 0	0.00000
HETATM	38 C	31.43046	44.54498	42.87772	C	0 0	0.00000
HETATM	39 C	33.39327	43.05017	43.13755	C	0 0	0.00000
HETATM	40 C	31.61535	42.51894	41.44798	C	0 0	0.00000
HETATM	41 H	37.79387	39.84120	40.85941	H	0 0	0.00000
HETATM	42 H	36.20337	43.70784	41.00294	H	0 0	0.00000
HETATM	43 H	37.86688	44.46282	42.76315	H	0 0	0.00000
HETATM	44 H	39.60893	42.76391	43.62921	H	0 0	0.00000
HETATM	45 H	38.31598	39.22387	36.11994	H	0 0	0.00000
HETATM	46 H	38.80514	40.53812	34.07482	H	0 0	0.00000
HETATM	47 H	38.23653	43.02663	33.99978	H	0 0	0.00000
HETATM	48 H	37.11271	44.09360	35.93786	H	0 0	0.00000
HETATM	49 H	37.66820	38.33092	37.66942	H	0 0	0.00000
HETATM	50 H	34.48547	35.38365	41.73953	H	0 0	0.00000
HETATM	51 H	35.99272	34.54877	39.92700	H	0 0	0.00000
HETATM	52 H	37.09174	36.19075	38.37039	H	0 0	0.00000
HETATM	53 H	36.08816	44.66759	37.38844	H	0 0	0.00000
HETATM	54 H	34.89849	46.54097	38.20792	H	0 0	0.00000
HETATM	55 H	33.26164	47.62497	39.76773	H	0 0	0.00000

HETATM	56 H	32.11792	46.27772	41.53402	H	0 0	0.00000
HETATM	57 H	35.46148	38.26053	43.85947	H	0 0	0.00000
HETATM	58 H	33.90639	39.09993	44.25822	H	0 0	0.00000
HETATM	59 H	34.97469	39.74116	42.93987	H	0 0	0.00000
HETATM	60 H	34.07938	36.09941	43.62263	H	0 0	0.00000
HETATM	61 H	32.68144	36.04085	42.47299	H	0 0	0.00000
HETATM	62 H	32.58021	37.04307	43.97283	H	0 0	0.00000
HETATM	63 H	31.99704	39.12244	42.57604	H	0 0	0.00000
HETATM	64 H	32.07821	38.10360	41.07914	H	0 0	0.00000
HETATM	65 H	33.07204	39.61317	41.19419	H	0 0	0.00000
HETATM	66 H	30.66216	44.99281	42.19013	H	0 0	0.00000
HETATM	67 H	31.95781	45.39235	43.39430	H	0 0	0.00000
HETATM	68 H	30.87697	43.96701	43.66599	H	0 0	0.00000
HETATM	69 H	32.84685	42.52683	43.96789	H	0 0	0.00000
HETATM	70 H	34.03619	43.84498	43.60340	H	0 0	0.00000
HETATM	71 H	34.08510	42.29994	42.66322	H	0 0	0.00000
HETATM	72 H	30.83436	42.92918	40.75358	H	0 0	0.00000
HETATM	73 H	31.09106	41.87854	42.20631	H	0 0	0.00000
HETATM	74 H	32.27900	41.84860	40.83416	H	0 0	0.00000
HETATM	75 Ru	41.26035	35.40462	39.49611	Ru	0 0	0.00000
HETATM	76 O	42.50795	35.99931	40.70653	O	0 0	0.00000
HETATM	77 O	40.70489	33.93821	40.48838	O	0 0	0.00000
HETATM	78 N	39.97148	36.50415	40.82809	N	0 0	0.00000
HETATM	79 N	41.60456	37.16693	38.26496	N	0 0	0.00000
HETATM	80 N	39.56557	35.15889	38.14552	N	0 0	0.00000
HETATM	81 C	39.54092	38.38938	42.25113	C	0 0	0.00000
HETATM	82 C	40.29669	37.73224	41.28273	C	0 0	0.00000
HETATM	83 C	38.89100	35.89893	41.37710	C	0 0	0.00000
HETATM	84 C	38.07825	36.47433	42.36000	C	0 0	0.00000
HETATM	85 C	38.40144	37.77841	42.84056	C	0 0	0.00000
HETATM	86 C	40.64071	37.20907	37.19078	C	0 0	0.00000
HETATM	87 C	40.75666	38.12058	36.09501	C	0 0	0.00000
HETATM	88 C	39.96618	38.01019	34.93079	C	0 0	0.00000
HETATM	89 C	38.92513	37.03654	34.88752	C	0 0	0.00000
HETATM	90 C	38.73465	36.18167	35.99610	C	0 0	0.00000
HETATM	91 C	39.60633	36.18892	37.12852	C	0 0	0.00000
HETATM	92 C	42.56800	37.97778	38.41425	C	0 0	0.00000
HETATM	93 C	43.61476	37.81235	39.39680	C	0 0	0.00000
HETATM	94 C	43.59367	36.81152	40.45011	C	0 0	0.00000
HETATM	95 C	44.76713	36.72184	41.28846	C	0 0	0.00000
HETATM	96 C	45.86299	37.59953	41.08654	C	0 0	0.00000
HETATM	97 C	45.85567	38.57165	40.05937	C	0 0	0.00000
HETATM	98 C	44.74865	38.66188	39.20336	C	0 0	0.00000
HETATM	99 C	38.69611	34.24013	38.18921	C	0 0	0.00000
HETATM	100 C	38.68587	33.17289	39.16778	C	0 0	0.00000
HETATM	101 C	37.63990	32.20581	39.01294	C	0 0	0.00000
HETATM	102 C	37.57784	31.10221	39.87849	C	0 0	0.00000
HETATM	103 C	38.56036	30.92926	40.88246	C	0 0	0.00000
HETATM	104 C	39.60318	31.87283	41.05678	C	0 0	0.00000
HETATM	105 C	39.68739	33.04874	40.21646	C	0 0	0.00000

HETATM	106	C	44.87712	35.71451	42.38543	C	0 0	0.00000
HETATM	107	C	43.74816	35.90910	43.41331	C	0 0	0.00000
HETATM	108	C	46.20730	35.81259	43.14864	C	0 0	0.00000
HETATM	109	C	44.75482	34.30356	41.78304	C	0 0	0.00000
HETATM	110	C	40.62773	31.60923	42.11092	C	0 0	0.00000
HETATM	111	C	40.34844	30.30598	42.87750	C	0 0	0.00000
HETATM	112	C	40.66211	32.75326	43.13760	C	0 0	0.00000
HETATM	113	C	42.01092	31.47888	41.44790	C	0 0	0.00000
HETATM	114	H	41.23998	38.16989	40.85975	H	0 0	0.00000
HETATM	115	H	38.68777	34.85722	41.00327	H	0 0	0.00000
HETATM	116	H	37.20190	35.92018	42.76325	H	0 0	0.00000
HETATM	117	H	37.80112	38.27900	43.62920	H	0 0	0.00000
HETATM	118	H	41.51365	38.92931	36.12008	H	0 0	0.00000
HETATM	119	H	40.13082	38.69517	34.07481	H	0 0	0.00000
HETATM	120	H	38.25999	36.95888	33.99943	H	0 0	0.00000
HETATM	121	H	37.89818	35.45282	35.93850	H	0 0	0.00000
HETATM	122	H	42.61179	38.81384	37.66993	H	0 0	0.00000
HETATM	123	H	46.75503	37.53274	41.73885	H	0 0	0.00000
HETATM	124	H	46.72297	39.25459	39.92591	H	0 0	0.00000
HETATM	125	H	44.75318	39.38560	38.36996	H	0 0	0.00000
HETATM	126	H	37.91325	34.27887	37.38888	H	0 0	0.00000
HETATM	127	H	36.88679	32.31230	38.20731	H	0 0	0.00000
HETATM	128	H	36.76559	30.35198	39.76633	H	0 0	0.00000
HETATM	129	H	38.50351	30.03484	41.53298	H	0 0	0.00000
HETATM	130	H	43.77598	36.93907	43.85953	H	0 0	0.00000
HETATM	131	H	43.82651	35.17280	44.25803	H	0 0	0.00000
HETATM	132	H	42.73693	35.77746	42.94017	H	0 0	0.00000
HETATM	133	H	46.33803	36.82292	43.62236	H	0 0	0.00000
HETATM	134	H	47.08782	35.64166	42.47290	H	0 0	0.00000
HETATM	135	H	46.27059	35.05294	43.97260	H	0 0	0.00000
HETATM	136	H	44.76129	33.50817	42.57599	H	0 0	0.00000
HETATM	137	H	45.60302	34.08761	41.07921	H	0 0	0.00000
HETATM	138	H	43.79898	34.19357	41.19420	H	0 0	0.00000
HETATM	139	H	40.34484	29.41690	42.18963	H	0 0	0.00000
HETATM	140	H	39.35084	30.33923	43.39400	H	0 0	0.00000
HETATM	141	H	41.12560	30.11558	43.66573	H	0 0	0.00000
HETATM	142	H	41.38847	32.54113	43.96791	H	0 0	0.00000
HETATM	143	H	39.65222	32.91272	43.60352	H	0 0	0.00000
HETATM	144	H	40.96640	33.72765	42.66356	H	0 0	0.00000
HETATM	145	H	42.04582	30.59725	40.75352	H	0 0	0.00000
HETATM	146	H	42.82744	31.34475	42.20643	H	0 0	0.00000
HETATM	147	H	42.26008	32.38885	40.83410	H	0 0	0.00000
HETATM	148	Ru	43.34936	43.38903	39.49560	Ru	0 0	0.00000
HETATM	149	O	42.21017	44.17257	40.70573	O	0 0	0.00000
HETATM	150	O	44.89741	43.64165	40.48908	O	0 0	0.00000
HETATM	151	N	43.04233	41.72276	40.82760	N	0 0	0.00000
HETATM	152	N	41.65144	42.80653	38.26540	N	0 0	0.00000
HETATM	153	N	44.41031	42.04339	38.14420	N	0 0	0.00000
HETATM	154	C	41.62510	40.40940	42.25117	C	0 0	0.00000
HETATM	155	C	41.81492	41.39119	41.28258	C	0 0	0.00000

HETATM	156	C	44.10668	41.08997	41.37683	C	0	0	0.00000
HETATM	157	C	44.01488	40.09890	42.35944	C	0	0	0.00000
HETATM	158	C	42.72300	39.72707	42.84062	C	0	0	0.00000
HETATM	159	C	42.09651	41.95135	37.19088	C	0	0	0.00000
HETATM	160	C	41.24968	41.59546	36.09486	C	0	0	0.00000
HETATM	161	C	41.74096	40.96581	34.93096	C	0	0	0.00000
HETATM	162	C	43.10456	40.55086	34.88785	C	0	0	0.00000
HETATM	163	C	43.93964	40.81369	35.99681	C	0	0	0.00000
HETATM	164	C	43.49781	41.56514	37.12851	C	0	0	0.00000
HETATM	165	C	40.46738	43.23611	38.41288	C	0	0	0.00000
HETATM	166	C	40.08746	44.22412	39.39600	C	0	0	0.00000
HETATM	167	C	40.96503	44.70666	40.44990	C	0	0	0.00000
HETATM	168	C	40.45529	45.76819	41.28872	C	0	0	0.00000
HETATM	169	C	39.14765	46.27776	41.08691	C	0	0	0.00000
HETATM	170	C	38.30868	45.78573	40.05997	C	0	0	0.00000
HETATM	171	C	38.78461	44.78161	39.20369	C	0	0	0.00000
HETATM	172	C	45.64116	41.75059	38.18985	C	0	0	0.00000
HETATM	173	C	46.56951	42.27491	39.16782	C	0	0	0.00000
HETATM	174	C	47.93034	41.85262	39.01300	C	0	0	0.00000
HETATM	175	C	48.91713	42.35123	39.87827	C	0	0	0.00000
HETATM	176	C	48.57584	43.28850	40.88210	C	0	0	0.00000
HETATM	177	C	47.23680	43.72003	41.05686	C	0	0	0.00000
HETATM	178	C	46.17612	43.20450	40.21659	C	0	0	0.00000
HETATM	179	C	41.27269	46.36645	42.38540	C	0	0	0.00000
HETATM	180	C	41.66872	45.29152	43.41335	C	0	0	0.00000
HETATM	181	C	40.52281	47.46951	43.14866	C	0	0	0.00000
HETATM	182	C	42.55576	46.96620	41.78313	C	0	0	0.00000
HETATM	183	C	46.95310	44.73906	42.11084	C	0	0	0.00000
HETATM	184	C	48.22113	45.14884	42.87756	C	0	0	0.00000
HETATM	185	C	45.94513	44.19698	43.13753	C	0	0	0.00000
HETATM	186	C	46.37463	46.00254	41.44845	C	0	0	0.00000
HETATM	187	H	40.96427	41.98899	40.85994	H	0	0	0.00000
HETATM	188	H	45.11058	41.43456	41.00292	H	0	0	0.00000
HETATM	189	H	44.93270	39.61657	42.76292	H	0	0	0.00000
HETATM	190	H	42.58943	38.95651	43.62961	H	0	0	0.00000
HETATM	191	H	40.17058	41.84654	36.12000	H	0	0	0.00000
HETATM	192	H	41.06435	40.76498	34.07502	H	0	0	0.00000
HETATM	193	H	43.50391	40.01345	34.00010	H	0	0	0.00000
HETATM	194	H	44.98888	40.45301	35.93868	H	0	0	0.00000
HETATM	195	H	39.72190	42.85745	37.66785	H	0	0	0.00000
HETATM	196	H	38.75854	47.08446	41.73973	H	0	0	0.00000
HETATM	197	H	37.28258	46.19560	39.92661	H	0	0	0.00000
HETATM	198	H	38.15505	44.42375	38.37036	H	0	0	0.00000
HETATM	199	H	45.99916	41.05264	37.38838	H	0	0	0.00000
HETATM	200	H	48.21429	41.14765	38.20733	H	0	0	0.00000
HETATM	201	H	49.97283	42.02299	39.76620	H	0	0	0.00000
HETATM	202	H	49.37890	43.68695	41.53285	H	0	0	0.00000
HETATM	203	H	40.76275	44.80068	43.85980	H	0	0	0.00000
HETATM	204	H	42.26736	45.72760	44.25793	H	0	0	0.00000
HETATM	205	H	42.28826	44.48163	42.93989	H	0	0	0.00000

HETATM	206	H	39.58217	47.07783	43.62293	H	0 0	0.00000
HETATM	207	H	40.23039	48.31789	42.47284	H	0 0	0.00000
HETATM	208	H	41.14919	47.90452	43.97275	H	0 0	0.00000
HETATM	209	H	43.24116	47.36953	42.57629	H	0 0	0.00000
HETATM	210	H	42.31846	47.80883	41.07928	H	0 0	0.00000
HETATM	211	H	43.12887	46.19321	41.19439	H	0 0	0.00000
HETATM	212	H	48.99306	45.59022	42.18980	H	0 0	0.00000
HETATM	213	H	48.69114	44.26826	43.39412	H	0 0	0.00000
HETATM	214	H	47.99741	45.91721	43.66579	H	0 0	0.00000
HETATM	215	H	45.76558	44.93197	43.96785	H	0 0	0.00000
HETATM	216	H	46.31184	43.24271	43.60336	H	0 0	0.00000
HETATM	217	H	44.94915	43.97330	42.66372	H	0 0	0.00000
HETATM	218	H	47.12053	46.47363	40.75408	H	0 0	0.00000
HETATM	219	H	46.08295	46.77655	42.20728	H	0 0	0.00000
HETATM	220	H	45.46196	45.76361	40.83499	H	0 0	0.00000
HETATM	221	C	33.80065	40.70124	38.19736	C	0 0	0.00000
HETATM	222	O	32.93315	40.42639	37.50026	O	0 0	0.00000
HETATM	223	C	42.49345	34.28192	38.19808	C	0 0	0.00000
HETATM	224	O	43.16642	33.66845	37.50212	O	0 0	0.00000
HETATM	225	C	43.70315	45.01570	38.19655	C	0 0	0.00000
HETATM	226	O	43.89657	45.90304	37.49731	O	0 0	0.00000

The torsional drives were performed over 100000 iterations with a timestep of 0.25 fs. The code is interpreted very much in the same way as that of the bond restraints. The first four number define the torsion, the next on is the starting angle, then the two forces and finally the change in torsion angle per iteration.

Propellor flip from **3b**-in:

TORSION RESTRAINT 8 2 81 82 73.55 2500.00 0.5000 -0.0007355
TORSION RESTRAINT 81 2 154 155 93.56 2500.00 0.5000 -0.0009356
TORSION RESTRAINT 154 2 8 9 71.40 2500.00 0.5000 -0.0007140

Propellor flip from **3b**-out:

TORSION RESTRAINT 8 2 81 82 107.88 2500.00 0.5000 -0.0010788
TORSION RESTRAINT 81 2 154 155 106.39 2500.00 0.5000 -0.0010639
TORSION RESTRAINT 154 2 8 9 97.95 2500.00 0.5000 -0.0009795

Propellor flip from **3g**-in:

TORSION RESTRAINT 8 2 81 82 58.63 2500.00 0.5000 -0.0005863
TORSION RESTRAINT 81 2 154 155 97.37 2500.00 0.5000 -0.0009737
TORSION RESTRAINT 154 2 8 9 98.61 2500.00 0.5000 -0.0009861

Propellor flip from **3g**-out:

TORSION RESTRAINT 8 2 81 82 107.56 2500.00 0.5000 -0.0010756
TORSION RESTRAINT 81 2 154 155 126.88 2500.00 0.5000 -0.0012688
TORSION RESTRAINT 154 2 8 9 127.09 2500.00 0.5000 -0.0012709

Salphen rotation from **3b**-in clockwise:

TORSION RESTRAINT 3 1 5 12 30.30 2500.00 0.5000 -0.0018000

Salphen rotation from **3b**-in counterclockwise:

TORSION RESTRAINT 3 1 5 12 30.30 2500.00 0.5000 0.0018000

Salphen rotation from **3b**-out clockwise:

TORSION RESTRAINT 3 1 5 9 41.79 2500.00 0.5000 -0.0018000

Salphen rotation from **3b**-out counterclockwise:

TORSION RESTRAINT 3 1 5 9 41.79 2500.00 0.5000 0.0018000

Salphen rotation from **3g**-in clockwise:

TORSION RESTRAINT 4 1 5 11 -31.33 2500.00 0.5000 -0.0018000

Salphen rotation from **3g**-in counterclockwise:

TORSION RESTRAINT 4 1 5 11 -31.33 2500.00 0.5000 0.0018000

Salphen rotation from **3g**-out clockwise:

TORSION RESTRAINT 4 1 5 10 -31.76 2500.00 0.5000 -0.0018000

Salphen rotation from **3g**-out counterclockwise:

TORSION RESTRAINT 4 1 5 10 -31.76 2500.00 0.5000 0.0018000

The starting points for the pyridine rotations were obtained in the same way, but in a different run, thus resulting in a different geometry. The rotation of the three pyridine rings to go from the in to the out conformation can be performed via many different pathways. This was explored exhaustively, but only the lowest energy pathways for the zinc and ruthenium complexes are presented in the paper. For the zinc complex **3b** this pathway started from the in conformation, and involved the simultaneous rotation of all three pyridine groups, of which two clockwise and one counterclockwise. The pathway is presented in reverse in figures 13 and 14. For the ruthenium complex **3g**, the lowest pathway was from out to in was found when one pyridine ring was driven clockwise and one counterclockwise. The third ring then rotated spontaneously.

Starting structure for pyridine rotation of **3b**:

HETATM	1 Zn	44.86981	42.93440	40.23051	Zn	1 0	0.00000
HETATM	2 P	40.11157	40.09849	40.66690	P	1 0	0.00000
HETATM	3 O	45.19153	41.02912	41.45455	O	2 0	0.00000
HETATM	4 O	45.70777	41.81531	38.61369	O	2 0	0.00000
HETATM	5 N	43.07726	42.57309	39.51702	N	2 0	0.00000
HETATM	6 N	44.27316	43.97871	41.86603	N	3 0	0.00000
HETATM	7 N	45.26613	44.78341	39.34925	N	3 0	0.00000
HETATM	8 C	40.98093	41.45703	39.66979	C	3 0	0.00000
HETATM	9 C	40.63216	41.84667	38.36081	C	3 0	0.00000
HETATM	10 C	41.57800	42.63008	37.63599	C	3 0	0.00000
HETATM	11 C	42.80610	42.96684	38.34059	C	3 0	0.00000
HETATM	12 C	42.23290	41.85021	40.20259	C	3 0	0.00000
HETATM	13 C	44.50766	45.32827	41.60964	C	3 0	0.00000
HETATM	14 C	45.05606	45.77163	40.29396	C	3 0	0.00000
HETATM	15 C	45.25340	47.17064	40.08387	C	3 0	0.00000
HETATM	16 C	44.86125	48.17391	41.01349	C	3 0	0.00000
HETATM	17 C	44.31497	47.68647	42.22067	C	3 0	0.00000

HETATM	18 C	44.21805	46.33283	42.58063	C	3 0	0.00000
HETATM	19 C	43.82647	43.38161	42.85577	C	4 0	0.00000
HETATM	20 C	43.51582	41.91613	42.94170	C	3 0	0.00000
HETATM	21 C	42.40720	41.61466	43.76538	C	3 0	0.00000
HETATM	22 C	41.81252	40.28870	43.79008	C	3 0	0.00000
HETATM	23 C	42.39271	39.24727	43.06472	C	3 0	0.00000
HETATM	24 C	43.62545	39.45127	42.36090	C	3 0	0.00000
HETATM	25 C	44.17919	40.78645	42.30019	C	3 0	0.00000
HETATM	26 C	45.58004	44.89815	38.15211	C	4 0	0.00000
HETATM	27 C	45.79503	43.79024	37.16419	C	3 0	0.00000
HETATM	28 C	45.75077	42.37502	37.37390	C	3 0	0.00000
HETATM	29 C	45.73552	41.51757	36.17914	C	3 0	0.00000
HETATM	30 C	45.92156	42.04373	34.88789	C	3 0	0.00000
HETATM	31 C	46.00333	43.45915	34.75218	C	3 0	0.00000
HETATM	32 C	45.97656	44.34516	35.87397	C	3 0	0.00000
HETATM	33 C	44.29563	38.35960	41.61901	C	4 0	0.00000
HETATM	34 C	45.75213	38.14635	42.07686	C	4 0	0.00000
HETATM	35 C	44.27002	38.60510	40.08936	C	4 0	0.00000
HETATM	36 C	43.55355	37.00790	41.85589	C	4 0	0.00000
HETATM	37 C	45.64929	40.05974	36.44289	C	4 0	0.00000
HETATM	38 C	45.64271	39.21360	35.14860	C	4 0	0.00000
HETATM	39 C	46.77102	39.53179	37.33954	C	4 0	0.00000
HETATM	40 C	44.28460	39.84202	37.12873	C	4 0	0.00000
HETATM	41 H	39.62841	41.54557	37.90807	H	1 0	0.00000
HETATM	42 H	41.34152	43.12130	36.68608	H	1 0	0.00000
HETATM	43 H	43.54895	43.60668	37.79339	H	1 0	0.00000
HETATM	44 H	42.51627	41.45936	41.26653	H	1 0	0.00000
HETATM	45 H	45.73986	47.39939	39.12706	H	1 0	0.00000
HETATM	46 H	44.95220	49.29773	40.79066	H	1 0	0.00000
HETATM	47 H	43.97326	48.47169	42.93150	H	1 0	0.00000
HETATM	48 H	43.77312	46.01256	43.55951	H	1 0	0.00000
HETATM	49 H	43.56205	44.03423	43.80396	H	1 0	0.00000
HETATM	50 H	41.87486	42.43524	44.29759	H	1 0	0.00000
HETATM	51 H	40.90766	40.06776	44.43273	H	1 0	0.00000
HETATM	52 H	41.91427	38.27345	43.09814	H	1 0	0.00000
HETATM	53 H	45.72245	45.93525	37.79287	H	1 0	0.00000
HETATM	54 H	45.92940	41.42492	33.99045	H	1 0	0.00000
HETATM	55 H	46.14068	44.02204	33.75506	H	1 0	0.00000
HETATM	56 H	46.03323	45.40066	35.68917	H	1 0	0.00000
HETATM	57 H	46.31287	39.13052	41.97551	H	1 0	0.00000
HETATM	58 H	46.21981	37.31307	41.45723	H	1 0	0.00000
HETATM	59 H	45.75536	37.85989	43.15286	H	1 0	0.00000
HETATM	60 H	44.74953	39.58084	39.89329	H	1 0	0.00000
HETATM	61 H	43.21816	38.69112	39.72232	H	1 0	0.00000
HETATM	62 H	44.79259	37.84490	39.47932	H	1 0	0.00000
HETATM	63 H	43.91504	36.22960	41.13157	H	1 0	0.00000
HETATM	64 H	42.46848	37.11193	41.60866	H	1 0	0.00000
HETATM	65 H	43.68103	36.61328	42.84777	H	1 0	0.00000
HETATM	66 H	44.90316	39.43538	34.40306	H	1 0	0.00000
HETATM	67 H	45.46551	38.12864	35.30050	H	1 0	0.00000

HETATM	68 H	46.62929	39.24366	34.65311	H	1 0	0.00000
HETATM	69 H	47.80812	39.73733	36.90568	H	1 0	0.00000
HETATM	70 H	46.67067	38.39747	37.50230	H	1 0	0.00000
HETATM	71 H	46.69127	39.89960	38.38066	H	1 0	0.00000
HETATM	72 H	44.31653	40.28023	38.14311	H	1 0	0.00000
HETATM	73 H	44.09205	38.72691	37.25104	H	1 0	0.00000
HETATM	74 H	43.38305	40.28813	36.60883	H	1 0	0.00000
HETATM	75 Zn	35.02434	42.51480	40.59606	Zn	1 0	0.00000
HETATM	76 O	36.30501	43.72331	41.87863	O	2 0	0.00000
HETATM	77 O	35.61964	43.83664	38.97683	O	2 0	0.00000
HETATM	78 N	36.30331	41.14858	39.79822	N	2 0	0.00000
HETATM	79 N	34.47910	41.58694	42.29229	N	3 0	0.00000
HETATM	80 N	33.27724	41.88103	39.82479	N	3 0	0.00000
HETATM	81 C	38.41606	40.22838	39.86484	C	3 0	0.00000
HETATM	82 C	38.28600	39.70922	38.53430	C	3 0	0.00000
HETATM	83 C	37.01611	39.84591	37.93318	C	3 0	0.00000
HETATM	84 C	36.06263	40.66905	38.64908	C	3 0	0.00000
HETATM	85 C	37.42647	41.01032	40.45747	C	3 0	0.00000
HETATM	86 C	33.28020	41.05871	42.10302	C	3 0	0.00000
HETATM	87 C	32.55856	41.24230	40.79486	C	3 0	0.00000
HETATM	88 C	31.29254	40.59755	40.60474	C	3 0	0.00000
HETATM	89 C	30.55434	39.99367	41.64925	C	3 0	0.00000
HETATM	90 C	31.21223	39.90786	42.86993	C	3 0	0.00000
HETATM	91 C	32.54392	40.36126	43.16650	C	3 0	0.00000
HETATM	92 C	35.25262	41.51042	43.27950	C	4 0	0.00000
HETATM	93 C	36.56848	42.09712	43.51400	C	3 0	0.00000
HETATM	94 C	37.33842	41.48404	44.58493	C	3 0	0.00000
HETATM	95 C	38.69063	41.77630	44.64869	C	3 0	0.00000
HETATM	96 C	39.35662	42.75907	43.86108	C	3 0	0.00000
HETATM	97 C	38.58575	43.45795	42.87221	C	3 0	0.00000
HETATM	98 C	37.17381	43.14630	42.74887	C	3 0	0.00000
HETATM	99 C	33.08630	42.12932	38.61793	C	4 0	0.00000
HETATM	100 C	33.90708	42.84487	37.57781	C	3 0	0.00000
HETATM	101 C	35.17315	43.58181	37.70635	C	3 0	0.00000
HETATM	102 C	35.84363	44.08351	36.53792	C	3 0	0.00000
HETATM	103 C	35.35208	43.81683	35.22861	C	3 0	0.00000
HETATM	104 C	34.17157	43.03345	35.08093	C	3 0	0.00000
HETATM	105 C	33.49051	42.54785	36.23842	C	3 0	0.00000
HETATM	106 C	39.20911	44.47977	41.95408	C	4 0	0.00000
HETATM	107 C	38.54084	45.83340	42.23088	C	4 0	0.00000
HETATM	108 C	38.90226	44.10453	40.48657	C	4 0	0.00000
HETATM	109 C	40.72111	44.56053	42.09177	C	4 0	0.00000
HETATM	110 C	37.12534	44.85109	36.80092	C	4 0	0.00000
HETATM	111 C	37.78416	45.25729	35.48676	C	4 0	0.00000
HETATM	112 C	36.73961	46.09004	37.61247	C	4 0	0.00000
HETATM	113 C	38.08927	43.85214	37.51461	C	4 0	0.00000
HETATM	114 H	39.09493	39.19256	37.97504	H	1 0	0.00000
HETATM	115 H	36.79234	39.48397	36.89188	H	1 0	0.00000
HETATM	116 H	35.08569	40.88732	38.08937	H	1 0	0.00000
HETATM	117 H	37.61295	41.59691	41.39082	H	1 0	0.00000

HETATM	118	H	30.73778	40.77440	39.68342	H	1	0	0.00000
HETATM	119	H	29.56476	39.64422	41.51665	H	1	0	0.00000
HETATM	120	H	30.68585	39.53096	43.74118	H	1	0	0.00000
HETATM	121	H	32.94649	40.30902	44.19341	H	1	0	0.00000
HETATM	122	H	34.86893	40.84879	44.06338	H	1	0	0.00000
HETATM	123	H	36.84869	40.74343	45.19281	H	1	0	0.00000
HETATM	124	H	39.34088	41.31312	45.47332	H	1	0	0.00000
HETATM	125	H	40.42168	42.84429	43.97658	H	1	0	0.00000
HETATM	126	H	32.07904	41.84432	38.28520	H	1	0	0.00000
HETATM	127	H	35.83490	44.28902	34.35196	H	1	0	0.00000
HETATM	128	H	33.81125	42.75659	34.05115	H	1	0	0.00000
HETATM	129	H	32.55311	41.96016	36.11624	H	1	0	0.00000
HETATM	130	H	37.44225	45.64096	42.37289	H	1	0	0.00000
HETATM	131	H	38.55061	46.54971	41.35219	H	1	0	0.00000
HETATM	132	H	39.00354	46.31186	43.15949	H	1	0	0.00000
HETATM	133	H	37.83407	44.00477	40.20980	H	1	0	0.00000
HETATM	134	H	39.31639	43.02200	40.36325	H	1	0	0.00000
HETATM	135	H	39.41668	44.72577	39.73915	H	1	0	0.00000
HETATM	136	H	41.13856	45.30029	41.36181	H	1	0	0.00000
HETATM	137	H	41.26538	43.59547	41.86954	H	1	0	0.00000
HETATM	138	H	41.05267	44.90440	43.07507	H	1	0	0.00000
HETATM	139	H	38.12705	44.35251	34.86210	H	1	0	0.00000
HETATM	140	H	38.67445	45.95853	35.64907	H	1	0	0.00000
HETATM	141	H	37.04832	45.83829	34.93049	H	1	0	0.00000
HETATM	142	H	35.84850	46.66824	37.26786	H	1	0	0.00000
HETATM	143	H	37.55464	46.79656	37.70298	H	1	0	0.00000
HETATM	144	H	36.46489	45.70653	38.61988	H	1	0	0.00000
HETATM	145	H	37.61789	43.25117	38.34601	H	1	0	0.00000
HETATM	146	H	38.98990	44.38152	37.91386	H	1	0	0.00000
HETATM	147	H	38.46347	43.05557	36.84380	H	1	0	0.00000
HETATM	148	Zn	40.03959	34.58702	40.46546	Zn	1	0	0.00000
HETATM	149	O	38.20505	35.15321	41.25540	O	2	0	0.00000
HETATM	150	O	39.01947	34.14916	38.65543	O	2	0	0.00000
HETATM	151	N	40.71030	36.28086	39.64020	N	2	0	0.00000
HETATM	152	N	40.85577	34.41183	42.40910	N	3	0	0.00000
HETATM	153	N	41.50675	33.13097	39.96089	N	3	0	0.00000
HETATM	154	C	40.72521	38.61893	39.71675	C	3	0	0.00000
HETATM	155	C	41.48732	38.71669	38.53567	C	3	0	0.00000
HETATM	156	C	41.76915	37.48795	37.87160	C	3	0	0.00000
HETATM	157	C	41.32107	36.26725	38.52320	C	3	0	0.00000
HETATM	158	C	40.38384	37.35252	40.26500	C	3	0	0.00000
HETATM	159	C	41.85956	33.44920	42.36672	C	3	0	0.00000
HETATM	160	C	42.22357	32.79783	41.13290	C	3	0	0.00000
HETATM	161	C	43.38891	31.94702	41.11711	C	3	0	0.00000
HETATM	162	C	44.14112	31.65371	42.26299	C	3	0	0.00000
HETATM	163	C	43.67645	32.13883	43.51146	C	3	0	0.00000
HETATM	164	C	42.58612	33.01635	43.54984	C	3	0	0.00000
HETATM	165	C	40.40789	35.13626	43.30833	C	4	0	0.00000
HETATM	166	C	39.28174	36.10623	43.22965	C	3	0	0.00000
HETATM	167	C	39.21416	37.07725	44.26022	C	3	0	0.00000

HETATM	168 C	38.13109	37.95500	44.33771	C	3 0	0.00000
HETATM	169 C	37.18097	38.04650	43.29216	C	3 0	0.00000
HETATM	170 C	37.14254	37.09206	42.24734	C	3 0	0.00000
HETATM	171 C	38.18558	36.08348	42.26356	C	3 0	0.00000
HETATM	172 C	41.68707	32.83960	38.77391	C	4 0	0.00000
HETATM	173 C	40.96200	33.30903	37.53498	C	3 0	0.00000
HETATM	174 C	39.71921	33.98268	37.50089	C	3 0	0.00000
HETATM	175 C	39.16291	34.50099	36.25751	C	3 0	0.00000
HETATM	176 C	39.87727	34.22328	35.04776	C	3 0	0.00000
HETATM	177 C	41.12553	33.56755	35.10039	C	3 0	0.00000
HETATM	178 C	41.61560	33.08021	36.32352	C	3 0	0.00000
HETATM	179 C	36.08508	37.08945	41.17819	C	4 0	0.00000
HETATM	180 C	35.30957	35.74895	41.14580	C	4 0	0.00000
HETATM	181 C	36.67436	37.17583	39.75323	C	4 0	0.00000
HETATM	182 C	35.14719	38.25217	41.44857	C	4 0	0.00000
HETATM	183 C	37.99474	35.40117	36.26301	C	4 0	0.00000
HETATM	184 C	37.47401	35.67087	34.83157	C	4 0	0.00000
HETATM	185 C	36.82388	34.86874	37.10711	C	4 0	0.00000
HETATM	186 C	38.45009	36.72540	36.92030	C	4 0	0.00000
HETATM	187 H	41.81392	39.70938	38.25251	H	1 0	0.00000
HETATM	188 H	42.35764	37.45855	36.93133	H	1 0	0.00000
HETATM	189 H	41.55521	35.29328	37.98822	H	1 0	0.00000
HETATM	190 H	39.84669	37.20705	41.23179	H	1 0	0.00000
HETATM	191 H	43.79192	31.37723	40.18755	H	1 0	0.00000
HETATM	192 H	44.99289	31.00834	42.21266	H	1 0	0.00000
HETATM	193 H	44.21619	31.84844	44.40894	H	1 0	0.00000
HETATM	194 H	42.41616	33.45846	44.59096	H	1 0	0.00000
HETATM	195 H	40.95989	35.07582	44.32433	H	1 0	0.00000
HETATM	196 H	39.99631	37.13419	45.08764	H	1 0	0.00000
HETATM	197 H	38.11312	38.74483	45.06479	H	1 0	0.00000
HETATM	198 H	36.44143	38.87161	43.21833	H	1 0	0.00000
HETATM	199 H	42.52347	32.08176	38.55246	H	1 0	0.00000
HETATM	200 H	39.59950	34.80191	34.15496	H	1 0	0.00000
HETATM	201 H	41.55724	33.28105	34.10767	H	1 0	0.00000
HETATM	202 H	42.57790	32.47653	36.31498	H	1 0	0.00000
HETATM	203 H	35.92591	34.90587	40.89335	H	1 0	0.00000
HETATM	204 H	34.41075	35.73645	40.44602	H	1 0	0.00000
HETATM	205 H	34.90329	35.49366	42.15698	H	1 0	0.00000
HETATM	206 H	37.55687	36.44612	39.71733	H	1 0	0.00000
HETATM	207 H	37.02943	38.22188	39.67856	H	1 0	0.00000
HETATM	208 H	35.89654	36.89070	38.97344	H	1 0	0.00000
HETATM	209 H	34.40798	38.41554	40.58755	H	1 0	0.00000
HETATM	210 H	35.72156	39.19402	41.66922	H	1 0	0.00000
HETATM	211 H	34.63880	38.07192	42.39564	H	1 0	0.00000
HETATM	212 H	38.26476	35.92054	34.08407	H	1 0	0.00000
HETATM	213 H	36.67773	36.46260	34.92924	H	1 0	0.00000
HETATM	214 H	36.94156	34.82976	34.42543	H	1 0	0.00000
HETATM	215 H	36.55889	33.85535	36.74356	H	1 0	0.00000
HETATM	216 H	35.93049	35.56008	37.13082	H	1 0	0.00000
HETATM	217 H	37.10252	34.64698	38.16901	H	1 0	0.00000

HETATM	218 H	38.86321	36.52826	37.95640	H	1 0 0.00000
HETATM	219 H	37.64155	37.52013	36.99542	H	1 0 0.00000
HETATM	220 H	39.27959	37.18872	36.34953	H	1 0 0.00000

Restraints for pyridine rotation of **3b**:

TORSION RESTRAINT	154	2	8 12	-93.83	2500.00	0.5000	0.001800
TORSION RESTRAINT	154	2	81 85	164.92	2500.00	0.5000	-0.001800
TORSION RESTRAINT	8	2	154 158	173.73	2500.00	0.5000	-0.001800

Starting structure for pyridine rotation of **3g**:

HETATM	1 Ru	35.05573	41.48872	39.85987	Ru	0 0 0.00000
HETATM	2 P	40.11720	40.06009	42.59589	P	0 0 0.00000
HETATM	3 O	35.11216	40.01083	40.99232	O	0 0 0.00000
HETATM	4 O	34.53711	42.81268	41.12442	O	0 0 0.00000
HETATM	5 N	36.86658	42.05826	40.95953	N	0 0 0.00000
HETATM	6 N	36.57143	40.62427	38.47554	N	0 0 0.00000
HETATM	7 N	35.41073	43.18736	38.51775	N	0 0 0.00000
HETATM	8 C	39.09729	41.36498	41.63415	C	0 0 0.00000
HETATM	9 C	37.87201	41.10088	41.06520	C	0 0 0.00000
HETATM	10 C	37.14382	43.28370	41.48208	C	0 0 0.00000
HETATM	11 C	38.42156	43.67418	41.95043	C	0 0 0.00000
HETATM	12 C	39.43368	42.69529	42.05197	C	0 0 0.00000
HETATM	13 C	37.15933	41.65237	37.62029	C	0 0 0.00000
HETATM	14 C	38.24486	41.47060	36.71568	C	0 0 0.00000
HETATM	15 C	38.60058	42.40811	35.73379	C	0 0 0.00000
HETATM	16 C	37.92169	43.65795	35.71081	C	0 0 0.00000
HETATM	17 C	36.87340	43.89012	36.62218	C	0 0 0.00000
HETATM	18 C	36.45324	42.92396	37.62319	C	0 0 0.00000
HETATM	19 C	36.88147	39.39006	38.49316	C	0 0 0.00000
HETATM	20 C	36.24782	38.42578	39.36817	C	0 0 0.00000
HETATM	21 C	35.25578	38.77997	40.41121	C	0 0 0.00000
HETATM	22 C	34.36738	37.70781	40.90542	C	0 0 0.00000
HETATM	23 C	34.64548	36.41537	40.39437	C	0 0 0.00000
HETATM	24 C	35.63788	36.15082	39.43128	C	0 0 0.00000
HETATM	25 C	36.48935	37.10049	38.84421	C	0 0 0.00000
HETATM	26 C	34.61306	44.21102	38.55089	C	0 0 0.00000
HETATM	27 C	33.54707	44.27519	39.49789	C	0 0 0.00000
HETATM	28 C	32.36864	44.93290	38.99735	C	0 0 0.00000
HETATM	29 C	31.27227	45.12549	39.82132	C	0 0 0.00000
HETATM	30 C	31.16520	44.41185	41.02499	C	0 0 0.00000
HETATM	31 C	32.27532	43.68677	41.61789	C	0 0 0.00000
HETATM	32 C	33.43871	43.53721	40.78222	C	0 0 0.00000
HETATM	33 C	33.20715	37.86321	41.79650	C	0 0 0.00000
HETATM	34 C	33.78960	38.16111	43.18844	C	0 0 0.00000
HETATM	35 C	32.37904	36.57907	42.01186	C	0 0 0.00000
HETATM	36 C	32.20219	38.91576	41.28070	C	0 0 0.00000
HETATM	37 C	32.32478	43.15032	42.98476	C	0 0 0.00000
HETATM	38 C	30.99981	43.11993	43.74687	C	0 0 0.00000
HETATM	39 C	33.24674	44.06506	43.81691	C	0 0 0.00000

HETATM	40 C	32.77501	41.67527	42.88640	C	0 0	0.00000
HETATM	41 H	37.58810	40.07366	40.69229	H	0 0	0.00000
HETATM	42 H	36.32848	44.05268	41.36987	H	0 0	0.00000
HETATM	43 H	38.70632	44.71435	42.22742	H	0 0	0.00000
HETATM	44 H	40.45385	42.96505	42.39780	H	0 0	0.00000
HETATM	45 H	38.82409	40.53905	36.72084	H	0 0	0.00000
HETATM	46 H	39.41775	42.17466	35.00203	H	0 0	0.00000
HETATM	47 H	38.30477	44.50269	35.09524	H	0 0	0.00000
HETATM	48 H	36.44085	44.93172	36.60659	H	0 0	0.00000
HETATM	49 H	37.66424	39.08531	37.76838	H	0 0	0.00000
HETATM	50 H	34.04965	35.49883	40.75608	H	0 0	0.00000
HETATM	51 H	35.77576	35.12431	39.06831	H	0 0	0.00000
HETATM	52 H	37.20485	36.91025	38.03323	H	0 0	0.00000
HETATM	53 H	34.66357	44.85207	37.64452	H	0 0	0.00000
HETATM	54 H	32.40031	45.35880	37.98109	H	0 0	0.00000
HETATM	55 H	30.45515	45.76322	39.38293	H	0 0	0.00000
HETATM	56 H	30.22435	44.52312	41.55799	H	0 0	0.00000
HETATM	57 H	34.37166	37.27091	43.55109	H	0 0	0.00000
HETATM	58 H	33.00277	38.35705	44.02511	H	0 0	0.00000
HETATM	59 H	34.46612	39.07094	43.06954	H	0 0	0.00000
HETATM	60 H	33.01632	35.79630	42.44956	H	0 0	0.00000
HETATM	61 H	31.94468	36.20658	41.08295	H	0 0	0.00000
HETATM	62 H	31.50786	36.74715	42.70518	H	0 0	0.00000
HETATM	63 H	31.38070	38.89996	42.04214	H	0 0	0.00000
HETATM	64 H	31.82641	38.69097	40.26356	H	0 0	0.00000
HETATM	65 H	32.64922	39.94087	41.22815	H	0 0	0.00000
HETATM	66 H	30.16491	42.72149	43.16190	H	0 0	0.00000
HETATM	67 H	30.64290	44.17850	44.02821	H	0 0	0.00000
HETATM	68 H	31.08017	42.53082	44.72210	H	0 0	0.00000
HETATM	69 H	33.52372	43.60070	44.81158	H	0 0	0.00000
HETATM	70 H	32.81346	45.10811	44.08107	H	0 0	0.00000
HETATM	71 H	34.17995	44.28503	43.20107	H	0 0	0.00000
HETATM	72 H	32.24389	41.12362	42.07026	H	0 0	0.00000
HETATM	73 H	32.38785	41.10335	43.75555	H	0 0	0.00000
HETATM	74 H	33.87719	41.51528	42.79593	H	0 0	0.00000
HETATM	75 Ru	41.23225	35.20264	39.41471	Ru	0 0	0.00000
HETATM	76 O	42.31742	35.94615	40.70270	O	0 0	0.00000
HETATM	77 O	40.73003	33.70484	40.41417	O	0 0	0.00000
HETATM	78 N	39.76954	36.31685	40.62539	N	0 0	0.00000
HETATM	79 N	41.63866	36.98790	38.21382	N	0 0	0.00000
HETATM	80 N	39.41634	35.01803	38.18150	N	0 0	0.00000
HETATM	81 C	39.46571	38.37129	41.88565	C	0 0	0.00000
HETATM	82 C	40.21914	37.58747	41.04078	C	0 0	0.00000
HETATM	83 C	38.55016	35.88766	40.96071	C	0 0	0.00000
HETATM	84 C	37.69475	36.69122	41.73484	C	0 0	0.00000
HETATM	85 C	38.13406	37.96017	42.23092	C	0 0	0.00000
HETATM	86 C	40.54100	37.14326	37.34857	C	0 0	0.00000
HETATM	87 C	40.29384	38.36737	36.60094	C	0 0	0.00000
HETATM	88 C	39.34377	38.50732	35.54429	C	0 0	0.00000
HETATM	89 C	38.53028	37.36767	35.28270	C	0 0	0.00000

HETATM	90 C	38.58741	36.27191	36.18804	C	0 0	0.00000
HETATM	91 C	39.53568	36.06683	37.23626	C	0 0	0.00000
HETATM	92 C	42.67567	37.73759	38.39271	C	0 0	0.00000
HETATM	93 C	43.72108	37.40261	39.32983	C	0 0	0.00000
HETATM	94 C	43.53967	36.56117	40.51514	C	0 0	0.00000
HETATM	95 C	44.67321	36.25311	41.36857	C	0 0	0.00000
HETATM	96 C	45.85935	36.95436	41.05802	C	0 0	0.00000
HETATM	97 C	46.01407	37.85072	39.98959	C	0 0	0.00000
HETATM	98 C	45.00438	38.03901	39.03635	C	0 0	0.00000
HETATM	99 C	38.57116	34.05080	38.24998	C	0 0	0.00000
HETATM	100 C	38.63480	32.97012	39.21309	C	0 0	0.00000
HETATM	101 C	37.52551	32.04660	39.05627	C	0 0	0.00000
HETATM	102 C	37.42714	30.97651	39.95917	C	0 0	0.00000
HETATM	103 C	38.51749	30.73625	40.83602	C	0 0	0.00000
HETATM	104 C	39.61279	31.62510	40.97931	C	0 0	0.00000
HETATM	105 C	39.65417	32.86987	40.21270	C	0 0	0.00000
HETATM	106 C	44.52496	35.31099	42.49163	C	0 0	0.00000
HETATM	107 C	45.79293	35.17933	43.35423	C	0 0	0.00000
HETATM	108 C	44.20747	33.90746	41.95034	C	0 0	0.00000
HETATM	109 C	43.37843	35.69029	43.44574	C	0 0	0.00000
HETATM	110 C	40.67804	31.29390	41.93601	C	0 0	0.00000
HETATM	111 C	40.53927	29.98199	42.72506	C	0 0	0.00000
HETATM	112 C	40.86274	32.42639	42.96662	C	0 0	0.00000
HETATM	113 C	41.97900	31.08740	41.10868	C	0 0	0.00000
HETATM	114 H	41.22216	37.92545	40.61800	H	0 0	0.00000
HETATM	115 H	38.27976	34.90978	40.54239	H	0 0	0.00000
HETATM	116 H	36.73592	36.30799	42.09920	H	0 0	0.00000
HETATM	117 H	37.45741	38.65153	42.76711	H	0 0	0.00000
HETATM	118 H	40.89425	39.26609	36.80869	H	0 0	0.00000
HETATM	119 H	39.30666	39.44668	34.92992	H	0 0	0.00000
HETATM	120 H	37.88886	37.32875	34.38874	H	0 0	0.00000
HETATM	121 H	37.73980	35.55813	36.01784	H	0 0	0.00000
HETATM	122 H	42.78725	38.68387	37.79902	H	0 0	0.00000
HETATM	123 H	46.78120	36.87375	41.72991	H	0 0	0.00000
HETATM	124 H	46.97256	38.42919	39.83671	H	0 0	0.00000
HETATM	125 H	45.16721	38.63612	38.14013	H	0 0	0.00000
HETATM	126 H	37.71921	34.10454	37.54214	H	0 0	0.00000
HETATM	127 H	36.80798	32.28369	38.24790	H	0 0	0.00000
HETATM	128 H	36.53201	30.30299	39.88056	H	0 0	0.00000
HETATM	129 H	38.43786	29.74390	41.40146	H	0 0	0.00000
HETATM	130 H	46.62868	34.78622	42.73800	H	0 0	0.00000
HETATM	131 H	45.61025	34.56793	44.29404	H	0 0	0.00000
HETATM	132 H	46.11106	36.23883	43.67282	H	0 0	0.00000
HETATM	133 H	45.04393	33.40140	41.44349	H	0 0	0.00000
HETATM	134 H	43.35218	33.99236	41.20769	H	0 0	0.00000
HETATM	135 H	43.88512	33.29286	42.82899	H	0 0	0.00000
HETATM	136 H	43.17929	34.91906	44.18032	H	0 0	0.00000
HETATM	137 H	42.41404	35.89402	42.89211	H	0 0	0.00000
HETATM	138 H	43.65744	36.66981	43.96685	H	0 0	0.00000
HETATM	139 H	40.37070	29.04040	42.12171	H	0 0	0.00000

HETATM	140	H	39.65809	30.10823	43.45101	H	0	0	0.00000
HETATM	141	H	41.46110	29.88233	43.29689	H	0	0	0.00000
HETATM	142	H	41.67259	32.11813	43.67418	H	0	0	0.00000
HETATM	143	H	39.92150	32.60338	43.53269	H	0	0	0.00000
HETATM	144	H	41.20042	33.43496	42.55289	H	0	0	0.00000
HETATM	145	H	42.87133	31.20519	41.81386	H	0	0	0.00000
HETATM	146	H	42.06809	31.80984	40.26778	H	0	0	0.00000
HETATM	147	H	42.05393	30.09559	40.57543	H	0	0	0.00000
HETATM	148	Ru	43.95709	43.25702	39.65478	Ru	0	0	0.00000
HETATM	149	O	42.52532	44.05670	40.67592	O	0	0	0.00000
HETATM	150	O	45.23609	43.35640	40.96336	O	0	0	0.00000
HETATM	151	N	43.39682	41.56365	40.78318	N	0	0	0.00000
HETATM	152	N	42.50564	42.21390	38.24375	N	0	0	0.00000
HETATM	153	N	45.33246	41.91921	38.51852	N	0	0	0.00000
HETATM	154	C	41.79133	40.08297	41.79626	C	0	0	0.00000
HETATM	155	C	42.12801	41.24977	41.05147	C	0	0	0.00000
HETATM	156	C	44.42550	40.72874	41.16875	C	0	0	0.00000
HETATM	157	C	44.18591	39.60836	41.99153	C	0	0	0.00000
HETATM	158	C	42.83697	39.25040	42.29544	C	0	0	0.00000
HETATM	159	C	43.22958	41.31905	37.38517	C	0	0	0.00000
HETATM	160	C	42.60154	40.55786	36.33067	C	0	0	0.00000
HETATM	161	C	43.31061	39.65132	35.50512	C	0	0	0.00000
HETATM	162	C	44.72005	39.60441	35.57508	C	0	0	0.00000
HETATM	163	C	45.42188	40.30426	36.60246	C	0	0	0.00000
HETATM	164	C	44.68745	41.16038	37.52400	C	0	0	0.00000
HETATM	165	C	41.21735	42.52000	38.30246	C	0	0	0.00000
HETATM	166	C	40.65582	43.68147	38.94378	C	0	0	0.00000
HETATM	167	C	41.38042	44.42922	40.03358	C	0	0	0.00000
HETATM	168	C	40.75802	45.69105	40.43784	C	0	0	0.00000
HETATM	169	C	39.46321	45.97981	40.01926	C	0	0	0.00000
HETATM	170	C	38.74584	45.18110	39.10556	C	0	0	0.00000
HETATM	171	C	39.33188	44.03726	38.52241	C	0	0	0.00000
HETATM	172	C	46.63820	42.07580	38.72427	C	0	0	0.00000
HETATM	173	C	47.21008	43.08784	39.54216	C	0	0	0.00000
HETATM	174	C	48.63031	43.30499	39.34097	C	0	0	0.00000
HETATM	175	C	49.24479	44.32775	40.07764	C	0	0	0.00000
HETATM	176	C	48.47530	45.08829	41.03175	C	0	0	0.00000
HETATM	177	C	47.10450	44.93902	41.29521	C	0	0	0.00000
HETATM	178	C	46.49795	43.82698	40.60018	C	0	0	0.00000
HETATM	179	C	41.43112	46.70804	41.30627	C	0	0	0.00000
HETATM	180	C	41.69470	46.35717	42.77611	C	0	0	0.00000
HETATM	181	C	40.59070	48.01228	41.29238	C	0	0	0.00000
HETATM	182	C	42.80379	47.10851	40.71094	C	0	0	0.00000
HETATM	183	C	46.33534	45.87617	42.19920	C	0	0	0.00000
HETATM	184	C	47.19461	45.93972	43.47070	C	0	0	0.00000
HETATM	185	C	44.97659	45.33785	42.67722	C	0	0	0.00000
HETATM	186	C	46.13364	47.22293	41.49104	C	0	0	0.00000
HETATM	187	H	41.35141	41.89672	40.56832	H	0	0	0.00000
HETATM	188	H	45.49049	40.95561	40.88341	H	0	0	0.00000
HETATM	189	H	45.08851	38.95928	42.23966	H	0	0	0.00000

HETATM	190	H	42.63574	38.27310	42.79611	H	0	0	0.00000
HETATM	191	H	41.51898	40.61547	36.20300	H	0	0	0.00000
HETATM	192	H	42.83814	39.00976	34.70512	H	0	0	0.00000
HETATM	193	H	45.21970	38.90865	34.88605	H	0	0	0.00000
HETATM	194	H	46.53753	40.23961	36.68324	H	0	0	0.00000
HETATM	195	H	40.60152	42.10682	37.45117	H	0	0	0.00000
HETATM	196	H	38.97724	46.92579	40.38217	H	0	0	0.00000
HETATM	197	H	37.70011	45.35067	38.83295	H	0	0	0.00000
HETATM	198	H	38.83803	43.47855	37.75989	H	0	0	0.00000
HETATM	199	H	47.28591	41.43349	38.10566	H	0	0	0.00000
HETATM	200	H	49.20054	42.75000	38.56124	H	0	0	0.00000
HETATM	201	H	50.31680	44.47549	39.86085	H	0	0	0.00000
HETATM	202	H	48.99849	45.83921	41.61602	H	0	0	0.00000
HETATM	203	H	42.39110	47.11705	43.24137	H	0	0	0.00000
HETATM	204	H	42.22307	45.36314	42.90136	H	0	0	0.00000
HETATM	205	H	40.82374	46.34841	43.44226	H	0	0	0.00000
HETATM	206	H	39.49985	47.82623	41.46612	H	0	0	0.00000
HETATM	207	H	40.70077	48.63279	40.34855	H	0	0	0.00000
HETATM	208	H	40.92327	48.66934	42.12349	H	0	0	0.00000
HETATM	209	H	43.56040	47.28834	41.50432	H	0	0	0.00000
HETATM	210	H	42.68079	48.01882	40.11224	H	0	0	0.00000
HETATM	211	H	43.22162	46.31388	40.06044	H	0	0	0.00000
HETATM	212	H	48.00843	46.69351	43.42496	H	0	0	0.00000
HETATM	213	H	47.65211	44.93916	43.71306	H	0	0	0.00000
HETATM	214	H	46.57094	46.22600	44.35643	H	0	0	0.00000
HETATM	215	H	44.56161	45.81460	43.59216	H	0	0	0.00000
HETATM	216	H	45.10532	44.27718	43.01894	H	0	0	0.00000
HETATM	217	H	44.18039	45.31491	41.93788	H	0	0	0.00000
HETATM	218	H	47.12870	47.74646	41.28088	H	0	0	0.00000
HETATM	219	H	45.44496	47.90143	42.08272	H	0	0	0.00000
HETATM	220	H	45.66227	47.13978	40.51124	H	0	0	0.00000
HETATM	221	C	33.52777	40.95313	38.74486	C	0	0	0.00000
HETATM	222	O	32.63651	40.58195	38.09983	O	0	0	0.00000
HETATM	223	C	42.23872	34.07275	38.07000	C	0	0	0.00000
HETATM	224	O	42.83063	33.38197	37.36679	O	0	0	0.00000
HETATM	225	C	44.47317	44.76890	38.47164	C	0	0	0.00000
HETATM	226	O	44.72001	45.66699	37.79563	O	0	0	0.00000

Restraints for pyridine rotation of **3g**:

TORSION RESTRAINT 81 2 8 12 178.98 2500.00 0.5000 -0.001800

TORSION RESTRAINT 154 2 81 85 -178.15 2500.00 0.5000 0.001800