Supplementary Material

EXAFS and EPR Studies of the Alkene Oxidation Catalyst Species, *trans*-[Cr^{III}(bpb)(L)₂]ⁿ⁺ and Cr(V) Oxidation Products (bpb = N,N'-Bis(2-pyridinecarboxamido)-1,2-benzene)

Colin L. Weeks, ^{A,B} Aviva Levina, ^A Ronald R. Fenton^A and Peter A. Lay^{A,C}*

- ^A School of Chemistry, The University of Sydney, NSW 2006, Australia
- ^B Current Address: Department of Chemistry and Biochemistry, University of Northern Iowa, Cedar Falls, IA 50614-0423, U.S.A.
- ^C Corresponding author. Email: <u>peter.lay@sydney.edu.au</u>

Wavenumber (cm^{-1})					
1.DMF.0.5H ₂ O	1 .H ₂ O	2	Assignment		
	3400-2700	3400-2400	vO–H		
3061			vC-H		
2941			vC-H		
1626	1615	1610	amide I		
1596	1591	1585	aromatic ring		
1574	1561	1544	skeletal vibrations		
1474	1473	1469	and C–H		
1450	1449	1450	deformations		
		1116	vCl–O		
811	807	803	coordinated H ₂ O rock		
755	754	754	C–H deformation		

 Table S1. Characteristic IR bands of 1 and 2

The sharp band due to the N–H stretch (at 3320 cm⁻¹ for bpbH₂) was absent from the IR spectra of **1** and **2**, which showed that bpb was coordinated *via* the deprotonated amide N to the Cr. There was little difference in the position of most of the IR bands of **1** and **2**, though the position of the amide I band varied somewhat. This was probably because the amide group of the DMF of crystallization, which was in the sample of **1** produced by Method 1, also occurs in this region. The presence of the perchlorate counterion in **2** was confirmed by the vCl–O band at 1116 cm⁻¹. The band at ~810 cm⁻¹ in the IR spectra was evidence that H₂O was coordinated in both products. The vCr–Cl vibration in Cr(III) complexes has been reported in the range 303-375 cm⁻¹,^{(39-41]} and the band at ~320 cm⁻¹ (which was absent from the IR spectrum of $[Cr^{III}(bpb)(OH_2)_2]CIO_4$) may be due to vCr–Cl. However, as vCr–N vibrations also occur in the 300-400 cm⁻¹ region,^{(39-41]} the ligand in the second axial coordination site could not be unambiguously assigned from the low frequency region of the IR spectra, without isotopic substitution.

Molecular	m/z	Relative Intensity		
Formula		Calculated	Observed	
$C_{18}H_{12}N_4O_2Cr$	366	5.2	5	
	367	1.1	2	
	368	100	100	
	369	32.5	32	
	370	7.7	10	
	371	1.1	1	
$C_{37}H_{27}N_8O_5Cr_2$	765	10.1	14	
	766	5.5	6	
	767	100	100	
	768	65.4	68	
	769	26.6	29	
	770	7.5	11	

 Table S2. Observed and calculated molecular isotope distributions for positive-ion ES/MS data for 2

Calculation of Determinancy

Parts of the bpb ligand were constrained to be planar and the bond lengths and angles within the bpb ligand were restrained using data on the ligand structure from crystal structures of it bound to other metal ions.^[10,34-36] According to Binsted *et al.*,^[37] additional independent observations are generated by the inclusion of distance information. The number of additional independent observations is equal to:

$$D(N-2) + 1$$

Where D is the number of dimensions in which the refinement takes place (3 for the refinements in this paper), N is the number of atoms in the restrained unit of the molecule. For example, to include the effect of the bond length and angle restraints on the determinancy for Model **III**, the calculations are:

$$N_{idp} = \frac{2 \times 11.5 \times 4.0}{\pi} + [3(13-2)+1]$$

$$N_{idp} = 63$$

Parameters = 2+14+42

= 58

$$Determinancy = \frac{N_{idp}}{Parameters}$$
$$= 1.09$$

The C bonded to the axial O atom was not included in the refinement because, unlike the atoms in the bpb ligand, the bond length and angle data available do not allow tight restraints.

Restra	aints
$S_0^2 \approx 0.9 \{0.2\}$	$\sigma_1^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_2^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_3^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_4^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_5^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_6^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_7^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_8^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_9^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{10}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{11}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{12}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{13}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{14}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{15}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{16}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma^2_{17} > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{18}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{19}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{20}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{21}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{22}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{23}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{24}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{25}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{26}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_1^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_2^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_3^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_4^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_5^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_6^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_7 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_8^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_9 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{10}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_{11} < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{12}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_{13} < 0.03 \{0.01\} \text{ Å}^2$
$\sigma^2_{14} < 0.03 \{0.01\} \text{ Å}^2$	$\sigma_{15}^2 < 0.03 \{0.01\} \text{ Å}^2$
$\sigma^2_{16} < 0.03 \{0.01\} \text{ Å}^2$	$\sigma^2_{17} < 0.02 \{0.01\} \text{ Å}^2$
$\sigma^2_{18} < 0.03 \{0.01\} \text{ Å}^2$	$\sigma^2_{19} < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{20}^2 < 0.03 \{0.01\} \text{ Å}^2$	$\sigma^2_{21} < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{22}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_{23} < 0.03 \{0.01\} \text{ Å}^2$
$\sigma^2_{24} < 0.03 \{0.01\} \text{ Å}^2$	$\sigma^2_{25} < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{26}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_7^2 > (\sigma_2^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{13}^2 > (\sigma_7^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{14}^2 > (\sigma_{13}^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{17}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{18}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{20}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{21}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{19}^2 > (\sigma_{18}^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{11}^2 > (\sigma_9^2 + 0.001) \{0.0005\} \text{ Å}^2$
N1–C17 ≈ 1.35 {0.05} Å	N1–C21 ≈ 1.34 {0.05} Å
C17–C18 ≈ 1.38 {0.05} Å	C18–C19 ≈ 1.38 {0.05} Å
C19–C20 ≈ 1.36 {0.05} Å	C20–C21 ≈ 1.37 {0.05} Å
N2−C7 ≈ 1.41 {0.05} Å	N2–C9 ≈ 1.34 {0.05} Å
C9–O11 ≈ 1.23 {0.05} Å	C9–C17 ≈ 1.50 {0.05} Å
C7–C8 ≈ 1.42 {0.05} Å	C7–C13 ≈ 1.39 {0.05} Å
C13–C14 ≈ 1.38 {0.05} Å	C14–C15 ≈ 1.38 {0.05} Å
Cr0–O5 < 3.0 {0.1} Å	Cr0–O6 < 3.0 {0.1} Å
$N1-Cr0-N2 \approx 81 \{10\}^{\circ}$	N1–Cr0–N4 $\approx 108 \{10\}^{\circ}$
N2–Cr0–N3 ≈ 82 {10}°	Cr0–N1–C17 ≈ 112 {5}°

Table S3. Restraints used in MS fits of model Ia to the EXAFS data of 2^{a}

C17–N1–C21 ≈ 118 {5}° $Cr0-N1-C21 \approx 129 \{5\}^{\circ}$ $Cr0-N2-C7 \approx 114 \{5\}^{\circ}$ $Cr0-N2-C9 \approx 119 \{5\}^{\circ}$ N2–C9–O11 ≈ 129 {5}° $C7-N2-C9 \approx 126 \{5\}^{\circ}$ $N2-C9-C17 \approx 110 \{5\}^{\circ}$ $O11-C9-C17 \approx 120 \{5\}^{\circ}$ $N2-C7-C8 \approx 115 \{5\}^{\circ}$ $N2-C7-C13 \approx 126 \{5\}^{\circ}$ $C8-C7-C13 \approx 120 \{5\}^{\circ}$ N1–C17–C9 ≈ 117 {5}° $C9-C17-C18 \approx 121 \{5\}^{\circ}$ $N1-C17-C18 \approx 121 \{5\}^{\circ}$ $N1-C21-C20 \approx 122 \{5\}^{\circ}$ $C17-C18-C19 \approx 119 \{5\}^{\circ}$ C18–C19–C20 ≈ 119 {5}° C19–C20–C21 ≈ 119 {5}° $C7-C13-C14 \approx 120 \{5\}^{\circ}$ $C13-C14-C13 \approx 120 \{5\}^{\circ}$ $O5-Cr0-N1 > 80 \{1\}^{\circ}$ $O5-Cr0-N2 > 80 \{1\}^{\circ}$ $O5-Cr0-N3 > 80 \{1\}^{\circ}$ $O5-Cr0-N4 > 80 \{1\}^{\circ}$ $O6-Cr0-N1 > 80 \{1\}^{\circ}$ $O6-Cr0-N2 > 80 \{1\}^{\circ}$ $O6-Cr0-N3 > 80 \{1\}^{\circ}$ $O6-Cr0-N4 > 80 \{1\}^{\circ}$ Atoms restrained to be approximately coplanar:^b $((C7-C13)\times(C8-C13))^{(C14-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{\circ}.(C15-C13) \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C16-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(N2-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(N3-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C9-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C10-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(O11-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(O12-C13)} \approx 0 \{0.01\}^{\circ}$ $((N1-C17)\times(C18-C17))^{(C19-C17)} \approx 0 \{0.01\}^{\circ}$ $((N1-C17)\times(C18-C17))^{(C20-C17)} \approx 0 \{0.01\}^{\circ}$ $((N1-C17)\times(C18-C17))^{(C21-C17)} \approx 0 \{0.01\}^{\circ}$

^{*a*} The ranges of the restraints are given in parentheses. ^{*b*} The vector dot product of the vector from atom4-atom2 with the vector cross product of the vectors atom1-atom2 and atom3-atom2 is restrained to be zero.

Constra	lints
$\sigma_1^2 = \sigma_4^2$	$\sigma_2^2 = \sigma_3^2$
$\sigma_7^2 = \sigma_8^2$	$\sigma_{9}^{2} = \sigma_{10}^{2}$
$\sigma_{11}^2 = \sigma_{12}^2$	$\sigma_{13}^2 = \sigma_{16}^2$
$\sigma^{2}_{14} = \sigma^{2}_{15}$	$\sigma^{2}_{17} = \sigma^{2}_{22}$
$\sigma_{18}^2 = \sigma_{23}^2$	$\sigma_{19}^2 = \sigma_{24}^2$
$\sigma^{2}_{20} = \sigma^{2}_{25}$	$\sigma^2_{21} = \sigma^2_{26}$
x1 = x4	y1 = -y4
z1 = z4	$x^2 = x^3$
$y^2 = -y^3$	$z^2 = z^3$
x7 = x8	y7 = -y8
z7 = z8	x9 = x10
y9 = -y10	z9 = z10
x11 = x12	y11 = -y12
z11 = z12	x13 = x16
$y_{13} = -y_{16}$	z13 = z16
x14 = x15	y14 = -y15
z14 = z15	x17 = x22
$y_{17} = -y_{22}$	z17 = z22
x18 = x23	$y_{18} = -y_{23}$
z18 = z23	x19 = x24
y19 = -y24	z19 = z24
x20 = x25	y20 = -y25
z20 = z25	x21 = x26
y21 = -y26	z21 = z26

 Table S4. Constraints used in MS fit of model Ia to the EXAFS data of 2

 Constraints

Path	Atoms in MS pathway ^a	Degeneracy	$R^{\rm b}$ (Å)	Importance
No.	· ·	c .		factor ^c
1	Cr0→N2→Cr0	2	1.94	100
2	Cr0→O5→Cr0	1	1.95	49.9
3	Cr0→O6→Cr0	1	2.03	51.4
4	Cr0→N1→Cr0	2	2.07	96.2
5	Cr0→C7→Cr0	2	2.82	26.0
6	Cr0→C10→Cr0	2	2.87	44.6
7	Cr0→C22→Cr0	2	2.87	42.3
8	Cr0→C7→N2→Cr0	4	3.08	16.2
9	Cr0→C9→N2→Cr0	4	3.08	31.8
10	Cr0→C26→Cr0	2	3.10	32.8
11	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$	4	3.15	23.0
12	Cr0→O5→N3→Cr0	2	3.19	5.11
13	$Cr0 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$	2	3.23	4.77
14	Cr0→O6→N3→Cr0	2	3.26	10.5
15	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow Cr0$	4	3.26	38.5
16	Cr0→N4→N3→Cr0	4	3.28	10.1
17	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$	2	3.29	7.81
18	$Cr0 \rightarrow O5 \rightarrow N2 \rightarrow Cr0$	2	3.30	4.34
19	$Cr0 \rightarrow N2 \rightarrow C7 \rightarrow N2 \rightarrow Cr0$	2	3.35	2.73
20	Cr0→N4→O6→Cr0	4	3.37	10.0
21	$Cr0 \rightarrow N4 \rightarrow C26 \rightarrow N4 \rightarrow Cr0$	2	3.42	13.8
22	$Cr0 \rightarrow N1 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$	2	3.42	3.63
23	Cr0→C7→C8→Cr0	2	3.52	3.97
24	Cr0→C7→N3→Cr0	4	3.57	6.76
25	Cr0→C22→N3→Cr0	4	3.57	9.32
26	$Cr0 \rightarrow N4 \rightarrow O5 \rightarrow Cr0$	2	3.61	3.63
27	$Cr0 \rightarrow C17 \rightarrow C9 \rightarrow Cr0$	4	3.62	11.5
28	$Cr0 \rightarrow C10 \rightarrow N4 \rightarrow Cr0$	4	3.68	8.25
29	$Cr0 \rightarrow N1 \rightarrow O5 \rightarrow Cr0$	2	3.71	6.03
30	$Cr0 \rightarrow N4 \rightarrow N1 \rightarrow Cr0$	2	3.78	4.90
31	$Cr0 \rightarrow N3 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$	2	3.88	7.38
32	$Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow O5 \rightarrow Cr0$	1	3.89	3.47
33	$Cr0 \rightarrow O5 \rightarrow O6 \rightarrow Cr0$	2	3.94	13.4
34	$Cr0 \rightarrow N2 \rightarrow N4 \rightarrow Cr0$	4	3.96	27.0
35	$Cr0 \rightarrow O6 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$	4	3.97	4.28
36	$Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow O6 \rightarrow Cr0$	2	3.98	16.9
37	$Cr0 \rightarrow C8 \rightarrow O6 \rightarrow Cr0$	4	4.00	3.72
38	Cr0→N3→Cr0→N1→Cr0	4	4.01	32.1
39	Cr0→N4→Cr0→N3→Cr0	4	4.01	4.49
40	$Cr0 \rightarrow O6 \rightarrow Cr0 \rightarrow O6 \rightarrow Cr0$	1	4.06	3.35

Table S5. Details of the SS and MS paths obtained from the MS fit of model **Ia** to the EXAFS data of **2**

41	Cr0→C9→C7→Cr0	4	4.07	3.75
42	Cr0→O11→Cr0	2	4.07	20.2
43	Cr0→O12→C10→Cr0	4	4.09	43.1
44	Cr0→N1→Cr0→O6→Cr0	4	4.10	3.48
45	$Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C10 \rightarrow Cr0$	2	4.10	25.9
46	Cr0→C10→O6→Cr0	4	4.12	4.38
47	$Cr0 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$	4	4.14	4.84
48	Cr0→N4→Cr0→N4→Cr0	2	4.14	5.58
49	Cr0→C16→Cr0	2	4.17	10.7
50	Cr0→O11→N2→Cr0	4	4.17	26.6
51	$Cr0 \rightarrow C9 \rightarrow O5 \rightarrow Cr0$	4	4.18	3.20
52	Cr0→C13→C7→Cr0	4	4.18	21.0
53	$Cr0 \rightarrow C9 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$	4	4.19	27.4
54	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$	2	4.20	12.7
55	Cr0→C18→Cr0	2	4.20	17.4
56	$Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$	2	4.22	1.88
57	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$	4	4.22	5.95
58	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$	2	4.22	8.00
59	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow C17 \rightarrow Cr0$	2	4.22	6.36
60	$Cr0 \rightarrow C32 \rightarrow C22 \rightarrow Cr0$	4	4.23	33.8
61	$Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$	2	4.25	19.1
62	Cr0→N3→O12→N3→Cr0	2	4.27	10.1
63	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$	4	4.28	4.24
64	$Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$	4	4.30	13.0
65	$Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$	4	4.30	15.7
66	$Cr0 \rightarrow N4 \rightarrow C26 \rightarrow C22 \rightarrow Cr0$	4	4.30	5.18
67	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$	4	4.31	13.5
68	Cr0→C18→N1→Cr0	4	4.33	20.6
69	$Cr0 \rightarrow N3 \rightarrow C8 \rightarrow C10 \rightarrow Cr0$	4	4.33	3.12
70	$Cr0 \rightarrow C17 \rightarrow O5 \rightarrow Cr0$	4	4.34	3.30
71	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$	4	4.34	6.90
72	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$	4	4.35	3.15
73	$Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$	4	4.35	19.7
74	Cr0→C9→N3→Cr0	4	4.36	4.76
75	$Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$	4	4.37	2.19
76	$Cr0 \rightarrow C10 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$	4	4.37	5.69
77	$Cr0 \rightarrow C25 \rightarrow Cr0$	2	4.37	7.43
78	$Cr0 \rightarrow C7 \rightarrow N1 \rightarrow Cr0$	4	4.40	2.71
79	$Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$	4	4.41	14.1
80	$Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N4 \rightarrow Cr0$	4	4.42	3.03
81	$Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$	4	4.42	14.3
82	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	4	4.42	2.81
83	$Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$	4	4.42	4.29

84 $Cr0 \rightarrow N3 \rightarrow C16 \rightarrow N3 \rightarrow Cr0$ 2 4.43 4.67 85 $Cr0 \rightarrow N3 \rightarrow OS \rightarrow N3 \rightarrow Cr0$ 2 4.44 3.43 86 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow N2 \rightarrow Cr0$ 4 4.45 3.43 87 $Cr0 \rightarrow C26 \rightarrow N3 \rightarrow Cr0$ 4 4.45 2.60 88 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow Cc0$ 2 4.45 6.84 89 $Cr0 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$ 2 4.45 5.89 90 $Cr0 \rightarrow N4 \rightarrow C23 \rightarrow N4 \rightarrow Cr0$ 2 4.45 5.89 90 $Cr0 \rightarrow N4 \rightarrow C23 \rightarrow N4 \rightarrow Cr0$ 2 4.45 7.19 91 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.47 3.02 93 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 2 4.47 6.08 94 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 2 4.49 3.11 95 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 2 4.53 3.43 98 $Cr0 \rightarrow OC3 \rightarrow N2 \rightarrow Cr0$ 4 4.56 10.02 96 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 4 4.66 2.73						
85 Cr0→N3→O5→N3→Cr0 2 4.44 3.43 86 Cr0→C13→C7→N2→Cr0 4 4.45 6.84 87 Cr0→C26→N3→Cr0 4 4.45 2.60 88 Cr0→C26→N4→C26→Cr0 2 4.45 5.89 90 Cr0→N1→C20→N1→Cr0 2 4.45 5.89 90 Cr0→N4→C23→N4→Cr0 2 4.45 7.19 91 Cr0→C26→C25→N4→Cr0 4 4.47 3.02 93 Cr0→C26→C25→C26→Cr0 2 4.47 6.08 94 Cr0→N3→O6→N3→Cr0 2 4.49 3.11 95 Cr0→N3→N4→N3→Cr0 2 4.49 3.02 96 Cr0→N3→N2→N3→Cr0 2 4.49 3.02 96 Cr0→C18→C17→N1→Cr0 4 4.58 6.57 100 Cr0→N1→N2→N1→Cr0 4 4.64 10.5 102 Cr0→O11→C17→Cr0 4 4.64 10.5 102 Cr0→O11→C17→Cr0 4 4.66 2.73 103 Cr0→C2→N2→Cr0 4 4.70 2.07	84	Cr0→N3→C16→N3→Cr0	2	4.43	4.67	
86 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow N2 \rightarrow Cr0$ 4 4.45 6.84 87 $Cr0 \rightarrow C26 \rightarrow N3 \rightarrow Cr0$ 4 4.45 2.60 88 $Cr0 \rightarrow C13 \rightarrow C26 \rightarrow N4 \rightarrow C26 \rightarrow Cr0$ 2 4.45 5.89 90 $Cr0 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$ 2 4.45 7.19 91 $Cr0 \rightarrow N2 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.46 10.8 92 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.47 3.02 93 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 2 4.49 3.11 95 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 2 4.49 3.02 96 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 2 4.49 3.01 97 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 2 4.58 3.13 98 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 2 4.58 6.57 100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 4 4.58 6.57 100 $Cr0 \rightarrow N1 \rightarrow O5 \rightarrow N1 \rightarrow Cr0$ 4 4.64 10.5 102 $Cr0 \rightarrow O1 \rightarrow C17 \rightarrow Cr0$ 4 4.64 10.5 102 $Cr0 \rightarrow C10 \rightarrow N1 \rightarrow Cr0$ 4 4.67 <td< td=""><td>85</td><td>$Cr0 \rightarrow N3 \rightarrow O5 \rightarrow N3 \rightarrow Cr0$</td><td>2</td><td>4.44</td><td>3.43</td><td></td></td<>	85	$Cr0 \rightarrow N3 \rightarrow O5 \rightarrow N3 \rightarrow Cr0$	2	4.44	3.43	
87 $Cr0 \rightarrow C26 \rightarrow N3 \rightarrow Cr0$ 4 4.45 2.60 88 $Cr0 \rightarrow C26 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$ 2 4.45 6.84 89 $Cr0 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$ 2 4.45 7.19 90 $Cr0 \rightarrow N4 \rightarrow C23 \rightarrow N4 \rightarrow Cr0$ 2 4.45 7.19 91 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.46 10.8 92 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.47 3.02 93 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 2 4.49 3.01 94 $Cr0 \rightarrow N3 \rightarrow 06 \rightarrow N3 \rightarrow Cr0$ 2 4.49 3.02 96 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 4 4.50 10.0 97 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 2 4.53 3.43 98 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 2 4.58 3.13 99 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 4 4.66 2.73 100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 4 4.66 2.73 102 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow Cr0$ 4 4.66 2.73 103 $Cr0 \rightarrow C1 \rightarrow C7 \rightarrow Cr0$ 4 4.67 2.86<	86	$Cr0 \rightarrow C13 \rightarrow C7 \rightarrow N2 \rightarrow Cr0$	4	4.45	6.84	
88 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C26 \rightarrow Cr0$ 2 4.45 6.84 89 $Cr0 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$ 2 4.45 5.89 90 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 2 4.45 7.19 91 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.46 10.8 92 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.47 3.02 93 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 2 4.49 3.11 95 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 2 4.49 3.02 96 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 2 4.53 3.43 97 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 2 4.53 3.43 98 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 2 4.58 6.57 100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 4 4.64 10.5 102 $Cr0 \rightarrow O1 \rightarrow O1 \rightarrow Cr0$ 4 4.66 2.73 103 $Cr0 \rightarrow O1 \rightarrow O1 \rightarrow Cr0$ 4 4.66 2.73 104 $Cr0 \rightarrow C1 \rightarrow O1 \rightarrow Cr0$ 4 4.69 6.28 105 $Cr0 \rightarrow C1 \rightarrow O2 \rightarrow Cr0$ 4 4.70 1.96 </td <td>87</td> <td>$Cr0 \rightarrow C26 \rightarrow N3 \rightarrow Cr0$</td> <td>4</td> <td>4.45</td> <td>2.60</td> <td></td>	87	$Cr0 \rightarrow C26 \rightarrow N3 \rightarrow Cr0$	4	4.45	2.60	
89 $Cr0 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$ 2 4.45 5.89 90 $Cr0 \rightarrow N4 \rightarrow C23 \rightarrow N4 \rightarrow Cr0$ 2 4.45 7.19 91 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 4 4.46 10.8 92 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 2 4.47 6.08 94 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 2 4.49 3.11 95 $Cr0 \rightarrow N3 \rightarrow 06 \rightarrow N3 \rightarrow Cr0$ 2 4.49 3.02 96 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 2 4.53 3.43 98 $Cr0 \rightarrow O20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 2 4.58 6.57 100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 2 4.62 3.08 101 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow Cr0$ 2 4.62 3.08 101 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow Cr0$ 2 4.62 3.08 101 $Cr0 \rightarrow O1 \rightarrow C1 \rightarrow Cr0$ 2 4.67 2.86 102 $Cr0 \rightarrow O1 \rightarrow D1 \rightarrow Cr2 \rightarrow Cr0$ 4 4.66 2.73 103 $Cr0 \rightarrow C1 \rightarrow O1 \rightarrow Cr2 \rightarrow Cr0$ 4 4.69 6.28 104 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow Cr0$ 4 4.70 1.96	88	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C26 \rightarrow Cr0$	2	4.45	6.84	
90 $Cr0 \rightarrow N4 \rightarrow C23 \rightarrow N4 \rightarrow Cr0$ 24.457.1991 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4610.892 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.476.0894 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 24.493.1195 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 24.493.0296 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow C1 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O1 \rightarrow C17 \rightarrow Cr0$ 44.662.73104 $Cr0 \rightarrow C1 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C1 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C1 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow C1 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.713.08106 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08106 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.7710.2115 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C1 \rightarrow C7 $	89	$Cr0 \rightarrow N1 \rightarrow C20 \rightarrow N1 \rightarrow Cr0$	2	4.45	5.89	
91 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4610.892 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.473.0293 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.476.0894 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 24.493.1195 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 24.493.0296 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.583.1398 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N2 \rightarrow CR \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow CR \rightarrow Cr0$ 44.762.73111 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow CR \rightarrow Cr0$ 44.762.73112 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow CR \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow CR \rightarrow Cr0$ 44.7710.2115 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C1 \rightarrow OS \rightarrow Cr0 \rightarrow CR \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C$	90	$Cr0 \rightarrow N4 \rightarrow C23 \rightarrow N4 \rightarrow Cr0$	2	4.45	7.19	
92 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 44.473.0293 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.476.0894 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 24.493.1195 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 24.493.0296 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 24.583.1399 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.7710.2114 $Cr0 \rightarrow C2 \rightarrow N2 \rightarrow Cr0$ 44.7710.1115 $Cr0 \rightarrow C1 \rightarrow N4 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C1 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.812.77118 $Cr0 \rightarrow C1 \rightarrow Cr0 \rightarrow $	91	$Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$	4	4.46	10.8	
93 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.476.0894 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 24.493.1195 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 24.493.0296 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.623.08101 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O1 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.6410.5103 $Cr0 \rightarrow O1 \rightarrow C2 \rightarrow Cr0$ 44.662.73104 $Cr0 \rightarrow C1 \rightarrow C1 \rightarrow Cr0$ 44.696.28105 $Cr0 \rightarrow C1 \rightarrow O1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C1 \rightarrow O1 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C1 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 44.762.73115 $Cr0 \rightarrow N2 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C1 \rightarrow N4 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C1 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C1 \rightarrow N2 \rightarrow Cr0$ <td>92</td> <td>$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$</td> <td>4</td> <td>4.47</td> <td>3.02</td> <td></td>	92	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$	4	4.47	3.02	
94 $Cr0 \rightarrow N3 \rightarrow O6 \rightarrow N3 \rightarrow Cr0$ 24.493.1195 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 24.493.0296 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 24.583.1399 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.713.08106 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.713.08107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.713.08108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C2 \rightarrow N2 \rightarrow Cr0$ 44.762.73111 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 44.762.73112 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C17 \rightarrow N2 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C17 \rightarrow N2 \rightarrow Cr0$	93	$Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$	2	4.47	6.08	
95 $Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$ 24.493.0296 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 24.583.1399 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow C1 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C2 \rightarrow N2 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C2 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.812.71119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow$	94	Cr0→N3→O6→N3→Cr0	2	4.49	3.11	
96 $Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.5010.097 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 24.583.1399 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C1 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 44.702.07106 $Cr0 \rightarrow C1 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C1 \rightarrow Or \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 Cr	95	$Cr0 \rightarrow N3 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$	2	4.49	3.02	
97 $Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 24.533.4398 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 24.583.1399 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.762.73112 $Cr0 \rightarrow C1 \rightarrow N4 \rightarrow Cr0$ 44.762.73113 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 44.7710.2115 $Cr0 \rightarrow C1 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C2 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C2 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C1 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C1 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C1 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ <	96	$Cr0 \rightarrow C18 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$	4	4.50	10.0	
98 $Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$ 24.583.1399 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.813.61120 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18$	97	$Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$	2	4.53	3.43	
99 $Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$ 44.586.57100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.8220.8	98	$Cr0 \rightarrow O6 \rightarrow N2 \rightarrow O6 \rightarrow Cr0$	2	4.58	3.13	
100 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 24.623.08101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.762.73112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.762.73113 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C17 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C70$ 44.813.56	99	$Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$	4	4.58	6.57	
101 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$ 44.6410.5102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C27 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	100	$Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	2	4.62	3.08	
102 $Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$ 44.662.73103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.7710.2115 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	101	$Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$	4	4.64	10.5	
103 $Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$ 24.672.86104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.762.73113 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	102	$Cr0 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$	4	4.66	2.73	
104 $Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$ 42.673.90105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.762.73113 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	103	$Cr0 \rightarrow O6 \rightarrow N1 \rightarrow O6 \rightarrow Cr0$	2	4.67	2.86	
105 $Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$ 44.696.28106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61123 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.56	104	$Cr0 \rightarrow C10 \rightarrow O12 \rightarrow C22 \rightarrow Cr0$	4	2.67	3.90	
106 $Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$ 44.702.07107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.765.27114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61123 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$ 44.813.56	105	$Cr0 \rightarrow C8 \rightarrow N1 \rightarrow Cr0$	4	4.69	6.28	
107 $Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$ 44.701.96108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.812.77119 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	106	$Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$	4	4.70	2.07	
108 $Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$ 24.702.84109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	107	$Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$	4	4.70	1.96	
109 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$ 44.713.08110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C22 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	108	$Cr0 \rightarrow N4 \rightarrow O6 \rightarrow N4 \rightarrow Cr0$	2	4.70	2.84	
110 $Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$ 44.711.72111 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	109	$Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$	4	4.71	3.08	
111 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$ 44.716.10112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.812.77118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.8112.2120 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	110	$Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$	4	4.71	1.72	
112 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$ 44.722.50113 $Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.8112.2120 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	111	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$	4	4.71	6.10	
113 $Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.762.73114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 44.765.27115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C24 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.8112.2120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	112	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C8 \rightarrow Cr0$	4	4.72	2.50	
114 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$ 4 4.76 5.27 115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 4 4.77 10.2 116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 4 4.77 6.11 117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.78 2.86 118 $Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 4 4.81 2.77 119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 2 4.81 12.2 120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 4 4.81 3.61 121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.81 3.61 122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.81 3.61 122 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.81 3.61 123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 4 4.82 20.8	113	$Cr0 \rightarrow C8 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$	4	4.76	2.73	
115 $Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$ 44.7710.2116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.8112.2120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.61121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	114	$Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$	4	4.76	5.27	
116 $Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$ 44.776.11117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.782.86118 $Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 44.812.77119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 24.8112.2120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.817.01121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 44.813.61122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 44.813.56123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 44.8220.8	115	$Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$	4	4.77	10.2	
117 $Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.78 2.86 118 $Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$ 4 4.81 2.77 119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 2 4.81 12.2 120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 4 4.81 7.01 121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.81 3.61 122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 4 4.81 3.61 122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 4 4.81 3.56 123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 4 4.82 20.8	116	$Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$	4	4.77	6.11	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	117	$Cr0 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$	4	4.78	2.86	
119 $Cr0 \rightarrow C24 \rightarrow Cr0$ 2 4.81 12.2 120 $Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 4 4.81 7.01 121 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$ 4 4.81 3.61 122 $Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$ 4 4.81 3.61 123 $Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$ 4 4.82 20.8	118	$Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$	4	4.81	2.77	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	119	$Cr0 \rightarrow C24 \rightarrow Cr0$	2	4.81	12.2	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	120	$Cr0 \rightarrow C17 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$	4	4.81	7.01	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	121	$Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C9 \rightarrow Cr0$	4	4.81	3.61	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	122	$Cr0 \rightarrow C^{2}2 \rightarrow Cr0 \rightarrow N^{3} \rightarrow Cr0$	4	4.81	3.56	
	123	$Cr0 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$	4	4.82	20.8	
$124 \qquad \text{Cr}0 \rightarrow \text{N1} \rightarrow \text{Cr}0 \qquad 2 \qquad 4.83 \qquad 10.2$	124	$Cr0 \rightarrow N1 \rightarrow C10 \rightarrow N1 \rightarrow Cr0$	2	4.83	10.2	
$125 Cr0 \rightarrow 012 \rightarrow C10 \rightarrow C22 \rightarrow Cr0 \qquad 4 \qquad 4.84 \qquad 5.34$	125	$Cr0 \rightarrow 012 \rightarrow C10 \rightarrow C22 \rightarrow Cr0$	$\frac{2}{4}$	4 84	5 34	
$126 Cr0 \rightarrow C8 \rightarrow N2 \rightarrow N3 \rightarrow Cr0 \qquad 4 \qquad 4.86 \qquad 3.97$	126	$Cr0 \rightarrow C8 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$	4	4 86	3 27	

127	$Cr0 \rightarrow C22 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$	4	4.86	3.81
128	$Cr0 \rightarrow C9 \rightarrow O11 \rightarrow N1 \rightarrow Cr0$	4	4.86	4.28
129	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N4 \rightarrow Cr0$	4	4.86	6.91
130	$Cr0 \rightarrow C18 \rightarrow N2 \rightarrow Cr0$	4	4.87	3.08
131	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C10 \rightarrow Cr0$	4	4.87	2.58
132	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C8$	4	4.88	2.60
133	$Cr0 \rightarrow C7 \rightarrow Cr0 \rightarrow N4 \rightarrow Cr0$	4	4.89	3.92
134	$Cr0 \rightarrow C13 \rightarrow C7 \rightarrow C8 \rightarrow Cr0$	4	4.89	2.38
135	$Cr0 \rightarrow C9 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$	4	4.89	4.18
136	$Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N2 \rightarrow Cr0$	4	4.89	4.05
137	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N3 \rightarrow Cr0$	4	4.90	2.78
138	$Cr0 \rightarrow C8 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	4	4.90	2.38
139	$Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N1 \rightarrow Cr0$	4	4.90	4.69
140	$Cr0 \rightarrow N4 \rightarrow C9 \rightarrow Cr0$	4	4.91	15.1
141	$Cr0 \rightarrow C21 \rightarrow N1 \rightarrow O5 \rightarrow Cr0$	4	4.91	4.19
142	$Cr0 \rightarrow C22 \rightarrow N3 \rightarrow N4 \rightarrow Cr0$	4	4.91	4.43
143	$Cr0 \rightarrow N3 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$	4	4.92	3.70
144	$Cr0 \rightarrow N4 \rightarrow Cr0 \rightarrow C9 \rightarrow Cr0$	4	4.94	16.8
145	$Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N1 \rightarrow Cr0$	4	4.94	3.13
146	$Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N1 \rightarrow Cr0$	4	3.94	6.87
147	$Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C17 \rightarrow Cr0$	4	4.95	2.02
148	$Cr0 \rightarrow N4 \rightarrow C7 \rightarrow N2 \rightarrow Cr0$	4	4.95	2.60
149	$Cr0 \rightarrow N4 \rightarrow C26 \rightarrow C10 \rightarrow Cr0$	4	4.97	3.46
150	$Cr0 \rightarrow C20 \rightarrow C17 \rightarrow Cr0$	4	4.98	1.26
151	$Cr0 \rightarrow N2 \rightarrow C26 \rightarrow Cr0$	4	4.99	12.6
152	$Cr0 \rightarrow N1 \rightarrow C20 \rightarrow C17 \rightarrow Cr0$	4	5.02	1.41
153	$Cr0 \rightarrow C24 \rightarrow C22 \rightarrow Cr0$	4	5.03	8.84
154	$Cr0 \rightarrow N3 \rightarrow Cr0 \rightarrow C21 \rightarrow Cr0$	4	5.04	12.5
155	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N3 \rightarrow Cr0$	4	5.04	2.48
156	$Cr0 \rightarrow C17 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$	4	5.04	7.36
157	$Cr0 \rightarrow N4 \rightarrow C22 \rightarrow N1 \rightarrow Cr0$	4	5.05	3.18
158	$Cr0 \rightarrow C26 \rightarrow Cr0 \rightarrow O5 \rightarrow Cr0$	4	5.05	1.81
159	$Cr0 \rightarrow C10 \rightarrow N3 \rightarrow N1 \rightarrow Cr0$	4	5.10	7.55
160	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow N4 \rightarrow Cr0$	4	5.12	6.86
161	$Cr0 \rightarrow C24 \rightarrow C26 \rightarrow Cr0$	4	5.13	5.84
162	$Cr0 \rightarrow N1 \rightarrow C19 \rightarrow C21 \rightarrow Cr0$	4	5.14	5.36
163	$Cr0 \rightarrow N4 \rightarrow C26 \rightarrow N2 \rightarrow Cr0$	4	5.15	7.99
164	$Cr0 \rightarrow C14 \rightarrow Cr0$	2	5.16	4.82
165	$Cr0 \rightarrow C21 \rightarrow N1 \rightarrow N3 \rightarrow Cr0$	4	5.16	7.63
166	$Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C18 \rightarrow Cr0$	4	5.16	4.18
167	$Cr0 \rightarrow C22 \rightarrow C7 \rightarrow Cr0$	4	5.17	1.91
168	$Cr0 \rightarrow C26 \rightarrow Cr0 \rightarrow N4 \rightarrow Cr0$	4	5.17	2.23
169	$Cr0 \rightarrow C14 \rightarrow C7 \rightarrow Cr0$	4	5.18	8.25

170	$Cr0 \rightarrow C7 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$	2	5.19	0.64	
171	$Cr0 \rightarrow N3 \rightarrow C8 \rightarrow O12 \rightarrow Cr0$	4	5.19	2.14	
172	$Cr0 \rightarrow C17 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$	4	5.19	1.60	
173	$Cr0 \rightarrow C8 \rightarrow C15 \rightarrow C8 \rightarrow Cr0$	2	5.20	3.12	
174	$Cr0 \rightarrow C24 \rightarrow C23 \rightarrow Cr0$	4	5.20	4.01	
175	$Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C22 \rightarrow Cr0$	2	5.20	2.09	
176	$Cr0 \rightarrow C18 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$	4	5.20	3.53	
177	$Cr0 \rightarrow C19 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$	4	5.22	5.05	
178	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C13 \rightarrow Cr0$	4	5.23	2.77	
179	$Cr0 \rightarrow C7 \rightarrow O6 \rightarrow N2 \rightarrow Cr0$	4	5.23	2.24	
180	$Cr0 \rightarrow C25 \rightarrow C22 \rightarrow N4 \rightarrow Cr0$	4	5.26	1.83	
181	$Cr0 \rightarrow C19 \rightarrow C20 \rightarrow Cr0$	4	5.27	2.78	
182	$Cr0 \rightarrow C25 \rightarrow C24 \rightarrow N4 \rightarrow Cr0$	4	5.28	2.35	
183	$Cr0 \rightarrow O11 \rightarrow C9 \rightarrow O11 \rightarrow Cr0$	2	5.31	5.78	
184	$Cr0 \rightarrow O11 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$	4	5.31	6.62	
185	$Cr0 \rightarrow C24 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$	4	5.32	2.88	
186	$Cr0 \rightarrow C9 \rightarrow O6 \rightarrow N2 \rightarrow Cr0$	4	5.35	3.16	
187	$Cr0 \rightarrow C15 \rightarrow C16 \rightarrow Cr0$	4	5.35	4.30	
188	$Cr0 \rightarrow O5 \rightarrow N1 \rightarrow O5 \rightarrow Cr0$	2	5.36	2.57	
189	$Cr0 \rightarrow C15 \rightarrow C16 \rightarrow C8 \rightarrow Cr0$	4	5.37	4.17	
190	$Cr0 \rightarrow C14 \rightarrow C8 \rightarrow Cr0$	4	5.37	3.74	
191	$Cr0 \rightarrow C13 \rightarrow C14 \rightarrow C7 \rightarrow Cr0$	4	5.37	4.04	
192	$Cr0 \rightarrow C8 \rightarrow C14 \rightarrow C7 \rightarrow Cr0$	4	5.39	3.13	
193	$Cr0 \rightarrow C18 \rightarrow N1 \rightarrow C17 \rightarrow Cr0$	4	5.40	5.33	
194	$Cr0 \rightarrow C15 \rightarrow N3 \rightarrow Cr0$	4	5.41	3.59	
195	$Cr0 \rightarrow N2 \rightarrow O6 \rightarrow C26 \rightarrow Cr0$	4	5.43	2.43	
196	$Cr0 \rightarrow C7 \rightarrow C14 \rightarrow N2 \rightarrow Cr0$	4	5.43	3.55	
197	$Cr0 \rightarrow C13 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$	4	5.44	2.66	
198	$Cr0 \rightarrow C15 \rightarrow C8 \rightarrow N3 \rightarrow Cr0$	4	5.45	3.35	
199	$Cr0 \rightarrow C17 \rightarrow O6 \rightarrow N1 \rightarrow Cr0$	4	5.45	2.98	
200	$Cr0 \rightarrow C15 \rightarrow C16 \rightarrow N3 \rightarrow Cr0$	4	5.48	3.63	
201	$Cr0 \rightarrow C10 \rightarrow C9 \rightarrow Cr0$	2	5.48	2.59	
202	$Cr0 \rightarrow C10 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$	4	5.50	5.27	
203	$Cr0 \rightarrow C9 \rightarrow O5 \rightarrow N2 \rightarrow Cr0$	4	5.53	3.40	

^{*a*} The atom numbering scheme is shown in Figure 1. ^{*b*} R is the total distance travelled by the photoelectron divided by two. ^{*c*} The importance factor is the percent contribution of a path relative to the strongest MS path and includes Debye-Waller contributions.

atom	σ^2 (Å ²)	atom	$\sigma^2 (\text{\AA}^2)$
N1	0.0010(1)	N2	0.0011(1)
O5	0.0026(4)	O6	0.0010(1)
C7	0.021(1)	C9	0.0010(1)
011	0.0024(2)	C13	0.022(1)
C14	0.030(1)	C17	0.0026(3)
C18	0.0020(1)	C19	0.0030(6)
C20	0.031(1)	C21	0.0037(4)

Table S6. Debye-Waller factors for model Ia of 2^a

^{*a*} The Monte-Carlo errors in the last significant figure are given in parentheses.

Restra	ints
$S_0^2 \approx 0.9 \{0.2\}$	$\sigma_1^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_2^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_3^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_4^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_5^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_6^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_7^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_8^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_9^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{10}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{11}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{12}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{13}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{14}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{15}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{16}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma^2_{17} > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{18}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{19}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{20}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{21}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{22}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{23}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{24}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_{25}^2 > 0.001 \{0.0005\} \text{ Å}^2$
$\sigma_{26}^2 > 0.001 \{0.0005\} \text{ Å}^2$	$\sigma_1^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_2^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_3^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_4^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_5^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_6^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_7 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_8^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma^2_9 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{10}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_{11}^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{12}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_{13}^2 < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{14}^2 < 0.03 \{0.01\} \text{ Å}^2$	$\sigma_{15}^2 < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{16}^2 < 0.03 \{0.01\} \text{ Å}^2$	$\sigma^2_{17} < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{18}^2 < 0.03 \{0.01\} \text{ Å}^2$	$\sigma_{19}^2 < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{20}^2 < 0.03 \{0.01\} \text{ Å}^2$	$\sigma_{21}^2 < 0.02 \{0.01\} \text{ Å}^2$
$\sigma_{22}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_{23}^2 < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{24}^2 < 0.03 \{0.01\} \text{ Å}^2$	$\sigma_{25}^2 < 0.03 \{0.01\} \text{ Å}^2$
$\sigma_{26}^2 < 0.02 \{0.01\} \text{ Å}^2$	$\sigma_7^2 > (\sigma_2^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{13}^2 > (\sigma_7^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{14}^2 > (\sigma_{13}^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{17}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{18}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{20}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{21}^2 > (\sigma_1^2 + 0.001) \{0.0005\} \text{ Å}^2$
$\sigma_{19}^2 > (\sigma_{18}^2 + 0.001) \{0.0005\} \text{ Å}^2$	$\sigma_{11}^2 > (\sigma_9^2 + 0.001) \{0.0005\} \text{ Å}^2$
N1−C17 ≈ 1.35 {0.05} Å	N1–C21 ≈ 1.34 {0.05} Å
C17–C18 ≈ 1.38 {0.05} Å	C18–C19 ≈ 1.38 {0.05} Å
C19–C20 ≈ 1.36 {0.05} Å	C20–C21 ≈ 1.37 {0.05} Å
N2−C7 ≈ 1.41 {0.05} Å	N2−C9 ≈ 1.34 {0.05} Å
C9–O11 ≈ 1.23 {0.05} Å	C9–C17 ≈ 1.50 {0.05} Å
C7–C8 ≈ 1.42 {0.05} Å	C7–C13 ≈ 1.39 {0.05} Å
C13–C14 ≈ 1.38 {0.05} Å	C14–C15 ≈ 1.38 {0.05} Å
Cr0–O5 < 3.0 {0.1} Å	Cr0–Cl6 < 3.5 {0.1} Å
N1–Cr0–N2 $\approx 81 \{10\}^{\circ}$	N1–Cr0–N4 $\approx 108 \{10\}^{\circ}$
$N2-Cr0-N3 \approx 82 \{10\}^{\circ}$	$Cr0-N1-C17 \approx 112 \{5\}^{\circ}$

Table S7. Restraints used in MS fits of model **III** to the EXAFS data of $1 \cdot \text{DMF} \cdot 0.5 \text{H}_2\text{O}^a$

 $Cr0-N1-C21 \approx 129 \{5\}^{\circ}$ $C17-N1-C21 \approx 118 \{5\}^{\circ}$ $Cr0-N2-C7 \approx 114 \{5\}^{\circ}$ $Cr0-N2-C9 \approx 119 \{5\}^{\circ}$ $C7-N2-C9 \approx 126 \{5\}^{\circ}$ N2–C9–O11 ≈ 129 {5}° $N2-C9-C17 \approx 110 \{5\}^{\circ}$ $O11-C9-C17 \approx 120 \{5\}^{\circ}$ $N2-C7-C8 \approx 115 \{5\}^{\circ}$ $N2-C7-C13 \approx 126 \{5\}^{\circ}$ $C8-C7-C13 \approx 120 \{5\}^{\circ}$ N1–C17–C9 ≈ 117 {5}° $N1-C17-C18 \approx 121 \{5\}^{\circ}$ $C9-C17-C18 \approx 121 \{5\}^{\circ}$ N1-C21-C20 \approx 122 {5}° $C17-C18-C19 \approx 119 \{5\}^{\circ}$ C18–C19–C20 ≈ 119 {5}° C19–C20–C21 ≈ 119 {5}° $C7-C13-C14 \approx 120 \{5\}^{\circ}$ $C13-C14-C13 \approx 120 \{5\}^{\circ}$ $O5-Cr0-N1 > 80 \{1\}^{\circ}$ $O5-Cr0-N2 > 80 \{1\}^{\circ}$ $O5-Cr0-N4 > 80 \{1\}^{\circ}$ $O5-Cr0-N3 > 80 \{1\}^{\circ}$ $Cl6-Cr0-N1 > 80 \{1\}^{\circ}$ $Cl6-Cr0-N2 > 80 \{1\}^{\circ}$ $Cl6-Cr0-N3 > 80 \{1\}^{\circ}$ $Cl6-Cr0-N4 > 80 \{1\}^{\circ}$ Atoms restrained to be approximately coplanar:^b $((C7-C13)\times(C8-C13))^{(C14-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C15-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C16-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(N2-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(N3-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C9-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(C10-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(O11-C13)} \approx 0 \{0.01\}^{\circ}$ $((C7-C13)\times(C8-C13))^{(O12-C13)} \approx 0 \{0.01\}^{\circ}$ $((N1-C17)\times(C18-C17))^{(C19-C17)} \approx 0 \{0.01\}^{\circ}$ $((N1-C17)\times(C18-C17))^{(C20-C17)} \approx 0 \{0.01\}^{\circ}$ $((N1-C17)\times(C18-C17))^{(C21-C17)} \approx 0 \{0.01\}^{\circ}$

^{*a*} The ranges of the restraints are given in parentheses. ^{*b*} The vector dot product of the vector from atom4-atom2 with the vector cross product of the vectors atom1-atom2 and atom3-atom2 is restrained to be zero.

Constraints				
$\sigma_1^2 = \sigma_4^2$	$\sigma_2^2 = \sigma_3^2$			
$\sigma_7^2 = \sigma_8^2$	$\sigma_{9}^{2} = \sigma_{10}^{2}$			
$\sigma_{11}^2 = \sigma_{12}^2$	$\sigma_{13}^2 = \sigma_{16}^2$			
$\sigma_{14}^2 = \sigma_{15}^2$	$\sigma_{17}^2 = \sigma_{22}^2$			
$\sigma_{18}^2 = \sigma_{23}^2$	$\sigma_{19}^2 = \sigma_{24}^2$			
$\sigma^2_{20} = \sigma^2_{25}$	$\sigma^2_{21} = \sigma^2_{26}$			
x1 = x4	y1 = -y4			
z1 = z4	$x^2 = x^3$			
$y^{2} = -y^{3}$	$z^2 = z^3$			
x7 = x8	y7 = -y8			
z7 = z8	x9 = x10			
y9 = -y10	z9 = z10			
x11 = x12	y11 = -y12			
z11 = z12	x13 = x16			
y13 = -y16	z13 = z16			
x14 = x15	y14 = -y15			
z14 = z15	x17 = x22			
y17 = -y22	z17 = z22			
x18 = x23	$y_{18} = -y_{23}$			
z18 = z23	x19 = x24			
y19 = -y24	z19 = z24			
x20 = x25	y20 = -y25			
z20 = z25	x21 = x26			
y21 = -y26	z21 = z26			

Table S8. Constraints used in MS fits of model **III** to the EXAFS data of $1 \cdot DMF \cdot 0.5H_2O$ Constraints

Path	Atoms in MS pathway ^a	Degeneracy	$R^{\rm b}$ (Å)	Importance
No.	1 5	6 1		factor ^c
1	Cr0→O5→Cr0	1	1.91	100
2	Cr0→N3→Cr0	2	1.98	100
3	Cr0→N4→Cr0	2	2.07	98.0
4	Cr0→Cl6→Cr0	1	2.32	38.6
5	Cr0→C22→Cr0	2	2.86	28.6
6	Cr0→C7→Cr0	2	2.88	46.1
7	Cr0→C9→Cr0	2	2.88	46.9
8	Cr0→C26→Cr0	2	3.09	26.8
9	Cr0→C10→N3→Cr0	4	3.10	33.1
10	Cr0→C8→N3→Cr0	4	3.14	27.5
11	Cr0→C22→N4→Cr0	4	3.14	17.9
12	Cr0→N2→O5→Cr0	4	3.24	10.9
13	Cr0→C26→N4→Cr0	4	3.25	34.5
14	Cr0→N2→N3→Cr0	2	3.28	5.44
15	Cr0→N1→N2→Cr0	4	3.32	11.4
16	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$	2	3.32	8.10
17	Cr0→N3→C8→N3→Cr0	2	3.40	5.53
18	$Cr0 \rightarrow N4 \rightarrow C26 \rightarrow N4 \rightarrow Cr0$	2	3.41	13.1
19	$Cr0 \rightarrow N4 \rightarrow C22 \rightarrow N4 \rightarrow Cr0$	2	3.42	3.1
20	Cr0→Cl6→N3→Cr0	4	3.54	6.77
21	Cr0→N1→O5→Cr0	2	3.58	4.02
22	Cr0→C17→N2→Cr0	4	3.59	8.32
23	$Cr0 \rightarrow C8 \rightarrow C7 \rightarrow Cr0$	2	3.59	7.62
24	Cr0→Cl6→N4→Cr0	4	3.61	6.55
25	Cr0→C7→N3→Cr0	4	3.62	10.8
26	$Cr0 \rightarrow C10 \rightarrow C22 \rightarrow Cr0$	4	3.63	10.9
27	Cr0→N4→O5→Cr0	2	3.66	6.42
28	Cr0→C9→N1→Cr0	4	3.70	9.85
29	Cr0→N4→N1→Cr0	2	3.79	5.88
30	$Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow O5 \rightarrow Cr0$	1	3.83	4.16
31	$Cr0 \rightarrow N3 \rightarrow Cr0 \rightarrow O5 \rightarrow Cr0$	4	3.90	1.23
32	Cr0→N3→Cr0→N3→Cr0	2	3.97	7.70
33	Cr0→N3→N1→Cr0	4	4.00	28.8
34	$Cr0 \rightarrow C7 \rightarrow O5 \rightarrow Cr0$	4	4.01	5.67
35	$Cr0 \rightarrow C9 \rightarrow O5 \rightarrow Cr0$	4	4.04	5.45
36	Cr0→N3→Cr0→N1→Cr0	4	4.05	33.5
37	Cr0→N4→Cr0→N3→Cr0	4	4.05	4.95
38	Cr0→O11→Cr0	2	4.09	20.9
39	$Cr0 \rightarrow O11 \rightarrow C9 \rightarrow Cr0$	4	4.10	44.9
40	$Cr0 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$	4	4.11	5.68

Table S9. Details of the SS and MS paths obtained from the MS fit of model **III** to the EXAFS data of $1 \cdot DMF \cdot 0.5H_2O$

42Cr0→C26→C22→Cr044.143.3943Cr0→N1→Cr0→N1→Cr024.146.5244Cr0→C18→Cr024.1919.345Cr0→O5→C16→Cr024.208.6746Cr0→O12→N3→Cr044.2130.348Cr0→C23→N2→C22→Cr044.222.3550Cr0→C23→N2→C22→Cr024.229.3051Cr0→C16→Cr024.2311.452Cr0→C10→C16→Cr024.2311.453Cr0→C13→C7→Cr044.269.8554Cr0→C13→C7→Cr044.269.8555Cr0→C9→N2→C7→Cr024.2422.354Cr0→C13→C7→Cr024.269.8556Cr0→C7→C13→C7→Cr024.269.8556Cr0→N1→C21→Cr024.3110.360Cr0→C13→N2→Cr044.3218.161Cr0→C13→N2→Cr044.324.8563Cr0→N2→C9→Cr0→Cr044.336.2864Cr0→C13→N2→Cr044.375.1769Cr0→C13→N2→Cr044.375.1760Cr0→C13→N2→Cr044.393.0271Cr0→C25→N4→Cr044.393.0271Cr0→C25→N4→Cr044.433.5872Cr0→C13→N2→Cr044.433.5873Cr0→C13→N2→Cr044.433.5874Cr0→N2→C21→Cr04 <th>41</th> <th>$Cr0 \rightarrow C9 \rightarrow O11 \rightarrow C9 \rightarrow Cr0$</th> <th>2</th> <th>4.11</th> <th>30.2</th>	41	$Cr0 \rightarrow C9 \rightarrow O11 \rightarrow C9 \rightarrow Cr0$	2	4.11	30.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42	$Cr0 \rightarrow C26 \rightarrow C22 \rightarrow Cr0$	4	4.14	3.39
44 $Cr0 \rightarrow C18 \rightarrow Cr0$ 24.1919.345 $Cr0 \rightarrow O5 \rightarrow C16 \rightarrow Cr0$ 24.208.6746 $Cr0 \rightarrow O12 \rightarrow N3 \rightarrow Cr0$ 44.2130.347 $Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$ 44.2236.949 $Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$ 24.222.3550 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$ 24.223.3051 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C1 \Rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 44.3228.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.332.8365 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C25 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.333.5872 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5873 Cr	43	$Cr0 \rightarrow N1 \rightarrow Cr0 \rightarrow N1 \rightarrow Cr0$	2	4.14	6.52
45Cr0 \rightarrow O5 \rightarrow Cl6 \rightarrow Cr024.208.6746Cr0 \rightarrow O12 \rightarrow N3 \rightarrow Cr044.2026.647Cr0 \rightarrow C9 \rightarrow O11 \rightarrow N2 \rightarrow Cr044.2130.348Cr0 \rightarrow C22 \rightarrow Cr2 \rightarrow Cr044.2236.949Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr024.222.3550Cr0 \rightarrow C2 \rightarrow N2 \rightarrow C9 \rightarrow Cr024.229.3051Cr0 \rightarrow C16 \rightarrow Cr024.2311.452Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow Cl6 \rightarrow Cr024.2318.453Cr0 \rightarrow C1 \rightarrow Cr1 \rightarrow Cr024.2422.354Cr0 \rightarrow C1 \rightarrow Cr \rightarrow Cr0 \rightarrow Cr044.269.8556Cr0 \rightarrow C7 \rightarrow Cr3 \rightarrow C7 \rightarrow Cr044.269.8556Cr0 \rightarrow C7 \rightarrow Cr3 \rightarrow C7 \rightarrow Cr024.2311.0360Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr024.3110.360Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr044.3222.161Cr0 \rightarrow O11 \rightarrow D2 \rightarrow Cr044.3222.162Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr044.336.2864Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr044.3522.165Cr0 \rightarrow C25 \rightarrow Cr024.359.1966Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.375.1769Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.393.0271Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.393.0271Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.335.8376Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.393.0271Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr	44	Cr0→C18→Cr0	2	4.19	19.3
46Cr0 \rightarrow O12 \rightarrow N3 \rightarrow Cr044.2026.647Cr0 \rightarrow C9 \rightarrow O11 \rightarrow N2 \rightarrow Cr044.2130.348Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr044.2236.949Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr024.222.3550Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr024.229.3051Cr0 \rightarrow C16 \rightarrow Cr024.2311.253Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr024.2422.354Cr0 \rightarrow C1 \rightarrow C7 \rightarrow Cr044.269.8556Cr0 \rightarrow C7 \rightarrow Cr3 \rightarrow C7 \rightarrow Cr024.2623.257Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr024.2623.257Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr024.2623.257Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C21 \rightarrow Cr7 \rightarrow Cr024.3110.360Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr044.3222.161Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr044.3224.8563Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr044.336.2864Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr044.3423.765Cr0 \rightarrow C25 \rightarrow Cr0 \rightarrow Cr044.3522.167Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.3723.368Cr0 \rightarrow N2 \rightarrow Cr \rightarrow Cr044.393.0271Cr0 \rightarrow C25 \rightarrow Cr \rightarrow Cr044.393.0271Cr0 \rightarrow C25 \rightarrow N3 \rightarrow Cr044.393.6273Cr0 \rightarrow C25 \rightarrow N3 \rightarrow Cr044.335.874Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr044.333.3376Cr	45	Cr0→O5→Cl6→Cr0	2	4.20	8.67
47 $Cr0 \rightarrow C9 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 44.2130.348 $Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$ 44.2236.949 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 24.222.3550 $Cr0 \rightarrow C2 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$ 24.229.3051 $Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2318.452 $Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.2623.257 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 44.3218.160 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3218.161 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C27 \rightarrow Cr0$ 44.3218.163 $Cr0 \rightarrow C26 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.322.864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3522.166 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3522.167 $Cr0 \rightarrow C25 \rightarrow Cr0 \rightarrow C7 \rightarrow Cr0$ 44.393.6271 $Cr0 \rightarrow C2 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.393.6272 $Cr0 \rightarrow C2 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.393.6273 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow Cr0$ <td>46</td> <td>Cr0→O12→N3→Cr0</td> <td>4</td> <td>4.20</td> <td>26.6</td>	46	Cr0→O12→N3→Cr0	4	4.20	26.6
48 $Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$ 44.2236.949 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 24.222.3550 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$ 24.229.3051 $Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.2311.0.360 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.324.8564 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow Cr0$ 44.433.5875 $Cr0 \rightarrow C25 \rightarrow N3 \rightarrow Cr0$ 44.433.5876 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow Cr0$ 44.433.5876	47	$Cr0 \rightarrow C9 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$	4	4.21	30.3
49 $Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 24.222.3550 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$ 24.229.3051 $Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3522.167 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.433.5872 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C1 \rightarrow C1 \rightarrow Cr0$ 44.433.5873 $Cr0 \rightarrow C2 \rightarrow C2 \rightarrow C2 \rightarrow Cr0$ <td< td=""><td>48</td><td>$Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$</td><td>4</td><td>4.22</td><td>36.9</td></td<>	48	$Cr0 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$	4	4.22	36.9
50 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$ 24.229.3051 $Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2318.452 $Cr0 \rightarrow C5 \rightarrow Cr0 \rightarrow Cl6 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.2536.755 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.2623.257 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow 07 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow N2 \rightarrow 07 \rightarrow N2 \rightarrow Cr0$ 44.3218.161 $Cr0 \rightarrow 011 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.336.2863 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3723.365 $Cr0 \rightarrow C25 \rightarrow Cr0$ 44.3723.366 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.375.1767 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.48 <td>49</td> <td>$Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$</td> <td>2</td> <td>4.22</td> <td>2.35</td>	49	$Cr0 \rightarrow C22 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$	2	4.22	2.35
51 $Cr0 \rightarrow C16 \rightarrow Cr0$ 24.2318.452 $Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow Cl6 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.2536.755 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.394.5671 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5875 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5876 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.443.48 <td>50</td> <td>$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$</td> <td>2</td> <td>4.22</td> <td>9.30</td>	50	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C9 \rightarrow Cr0$	2	4.22	9.30
52 $Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow Cl6 \rightarrow Cr0$ 24.2311.253 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.269.8555 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.2623.257 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C2 \rightarrow Cr0$ 44.433.5873 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow Cr0$ 44.433.5874 $Cr0 \rightarrow N1 \rightarrow C1 \rightarrow Cr0$ 44.433.5875 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow Cr0$ 44.433.5876 $Cr0 \rightarrow C2 \rightarrow N3 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.44	51	Cr0→C16→Cr0	2	4.23	18.4
53 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$ 24.2422.354 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.2536.755 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 24.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C17 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow C2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.444.4679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 4<	52	$Cr0 \rightarrow O5 \rightarrow Cr0 \rightarrow Cl6 \rightarrow Cr0$	2	4.23	11.2
54 $Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 44.2536.755 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.2623.257 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow 011 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow N2 \rightarrow 011 \rightarrow N2 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow 011 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow 011 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C1 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.433.5874 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.433.5875 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5876 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.444.4679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 4<	53	$Cr0 \rightarrow C17 \rightarrow C18 \rightarrow C17 \rightarrow Cr0$	2	4.24	22.3
55 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 44.269.8556 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.2623.257 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.433.5875 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5876 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.443.4876 $Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.4513.277 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow$	54	$Cr0 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$	4	4.25	36.7
56 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$ 24.2623.257 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow 011 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow 011 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C17 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.4513.280 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2783 $Cr0 \rightarrow C26 \rightarrow C$	55	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$	4	4.26	9.85
57 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$ 24.297.7958 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.443.4879 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2783 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow$	56	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow C7 \rightarrow Cr0$	2	4.26	23.2
58 $Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$ 44.303.8359 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.3916.671 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.412.9574 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2783 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N2 \rightarrow N$	57	$Cr0 \rightarrow C7 \rightarrow N2 \rightarrow C7 \rightarrow Cr0$	2	4.29	7.79
59 $Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$ 24.3110.360 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4513.280 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	58	$Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C17 \rightarrow Cr0$	4	4.30	3.83
60 $Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3222.161 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C2 \rightarrow C2 \rightarrow C4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C2 \rightarrow C$	59	$Cr0 \rightarrow N2 \rightarrow O11 \rightarrow N2 \rightarrow Cr0$	2	4.31	10.3
61 $Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$ 44.3218.162 $Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$ 44.324.8563 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C17 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N1 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C2 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	60	$Cr0 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$	4	4.32	22.1
62Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr044.324.8563Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr044.336.2864Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr044.3423.765Cr0 \rightarrow C25 \rightarrow Cr024.359.1966Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.3522.167Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr044.3723.368Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr044.375.1769Cr0 \rightarrow C1 \rightarrow N2 \rightarrow Cr \rightarrow C9 \rightarrow Cr044.393.0271Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr044.393.0271Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr044.405.9573Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr044.412.9575Cr0 \rightarrow C1 \rightarrow N1 \rightarrow C21 \rightarrow Cr024.433.3376Cr0 \rightarrow C4 \rightarrow S \rightarrow N4 \rightarrow Cr024.443.4878Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr024.448.2380Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr044.4513.281Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr044.454.2782Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr024.467.3083Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr044.474.30	61	$Cr0 \rightarrow O11 \rightarrow C9 \rightarrow N2 \rightarrow Cr0$	4	4.32	18.1
63 $Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$ 44.336.2864 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.433.5876 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.4513.282 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	62	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$	4	4.32	4.85
64 $Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 44.3423.765 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3522.167 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C2r0$ 24.433.3376 $Cr0 \rightarrow C4 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.448.2381 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	63	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C7 \rightarrow Cr0$	4	4.33	6.28
65 $Cr0 \rightarrow C25 \rightarrow Cr0$ 24.359.1966 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3522.167 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	64	$Cr0 \rightarrow C17 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$	4	4.34	23.7
66 $Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3522.167 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	65	$Cr0 \rightarrow C25 \rightarrow Cr0$	2	4.35	9.19
67 $Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$ 44.3723.368 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.443.4877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	66	$Cr0 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$	4	4.35	22.1
68 $Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$ 44.375.1769 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	67	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$	4	4.37	23.3
69 $Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$ 44.394.5670 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.280 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	68	$Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C9 \rightarrow Cr0$	4	4.37	5.17
70 $Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$ 44.393.0271 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	69	$Cr0 \rightarrow C10 \rightarrow N2 \rightarrow Cr0$	4	4.39	4.56
71 $Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.3916.672 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	70	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N2 \rightarrow Cr0$	4	4.39	3.02
72 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$ 44.405.9573 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	71	$Cr0 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$	4	4.39	16.6
73 $Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 44.4016.374 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	72	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$	4	4.40	5.95
74 $Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$ 44.412.9575 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	73	$Cr0 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$	4	4.40	16.3
75 $Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$ 24.433.3376 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	74	$Cr0 \rightarrow N1 \rightarrow C17 \rightarrow C21 \rightarrow Cr0$	4	4.41	2.95
76 $Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$ 44.433.5877 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	75	$Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C21 \rightarrow Cr0$	2	4.43	3.33
77 $Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.443.4878 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	76	$Cr0 \rightarrow C8 \rightarrow N3 \rightarrow N2 \rightarrow Cr0$	4	4.43	3.58
78 $Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 24.446.9679 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	77	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	4	4.44	3.48
79 $Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$ 24.448.2380 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	78	$Cr0 \rightarrow N4 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$	2	4.44	6.96
80 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$ 44.4513.281 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	79	$Cr0 \rightarrow N1 \rightarrow C18 \rightarrow N1 \rightarrow Cr0$	2	4.44	8.23
81 $Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$ 44.454.2782 $Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$ 24.467.3083 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 44.474.30	80	$Cr0 \rightarrow C26 \rightarrow C25 \rightarrow N4 \rightarrow Cr0$	4	4.45	13.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	81	$Cr0 \rightarrow C8 \rightarrow N4 \rightarrow Cr0$	4	4.45	4.27
83 $Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$ 4 4.47 4.30	82	$Cr0 \rightarrow C26 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$	2	4.46	7.30
	83	$Cr0 \rightarrow C7 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	4	4.47	4.30

84	$Cr0 \rightarrow N2 \rightarrow C13 \rightarrow N2 \rightarrow Cr0$	2	4.48	8.07	
85	$Cr0 \rightarrow C21 \rightarrow N2 \rightarrow Cr0$	4	4.48	2.14	
86	$Cr0 \rightarrow C21 \rightarrow N4 \rightarrow Cr0$	4	4.48	1.94	
87	$Cr0 \rightarrow O5 \rightarrow N2 \rightarrow O5 \rightarrow Cr0$	2	4.49	3.59	
88	$Cr0 \rightarrow C23 \rightarrow C22 \rightarrow N4 \rightarrow Cr0$	4	4.49	11.8	
89	$Cr0 \rightarrow C26 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$	4	4.50	2.75	
90	$Cr0 \rightarrow C13 \rightarrow C7 \rightarrow N2 \rightarrow Cr0$	4	4.51	12.9	
91	$Cr0 \rightarrow C20 \rightarrow C21 \rightarrow N1 \rightarrow Cr0$	4	4.56	7.73	
92	$Cr0 \rightarrow N2 \rightarrow O5 \rightarrow N2 \rightarrow Cr0$	2	4.57	3.85	
93	Cr0→N3→N4→N3→Cr0	2	4.57	3.37	
94	$Cr0 \rightarrow N3 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$	2	4.58	3.69	
95	$Cr0 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$	4	4.63	3.76	
96	$Cr0 \rightarrow Cl6 \rightarrow Cr0 \rightarrow Cl6 \rightarrow Cr0$	1	4.64	1.40	
97	$Cr0 \rightarrow N1 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	2	4.65	3.40	
98	$Cr0 \rightarrow C22 \rightarrow N2 \rightarrow Cr0$	4	4.66	7.73	
99	Cr0→O12→C22→Cr0	4	4.66	2.95	
100	$Cr0 \rightarrow C9 \rightarrow O11 \rightarrow C17 \rightarrow Cr0$	4	4.68	4.14	
101	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow C17 \rightarrow Cr0$	4	4.71	5.51	
102	Cr0→C8→N1→Cr0	4	4.74	9.98	
103	$Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C8 \rightarrow Cr0$	4	4.74	2.31	
104	$Cr0 \rightarrow C10 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$	4	4.74	3.49	
105	$Cr0 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$	4	4.76	4.03	
106	$Cr0 \rightarrow C21 \rightarrow N1 \rightarrow O5 \rightarrow Cr0$	2	4.76	1.58	
107	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow C9 \rightarrow Cr0$	4	4.77	4.73	
108	$Cr0 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$	4	4.77	7.90	
109	$Cr0 \rightarrow C8 \rightarrow N3 \rightarrow C7 \rightarrow Cr0$	4	4.78	6.67	
110	$Cr0 \rightarrow C8 \rightarrow C16 \rightarrow C7 \rightarrow Cr0$	4	4.78	4.97	
111	$Cr0 \rightarrow C23 \rightarrow C10 \rightarrow Cr0$	4	4.79	3.54	
112	Cr0→C19→Cr0	2	4.79	13.5	
113	$Cr0 \rightarrow N1 \rightarrow C21 \rightarrow O5 \rightarrow Cr0$	4	4.79	2.31	
114	$Cr0 \rightarrow C24 \rightarrow N4 \rightarrow Cr0$	4	4.80	23.1	
115	$Cr0 \rightarrow C22 \rightarrow C23 \rightarrow C10 \rightarrow Cr0$	4	4.81	4.06	
116	$Cr0 \rightarrow N1 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$	2	4.81	12.4	
117	$Cr0 \rightarrow N4 \rightarrow Cl6 \rightarrow N2 \rightarrow Cr0$	4	4.83	3.35	
118	$Cr0 \rightarrow C25 \rightarrow N4 \rightarrow O5 \rightarrow Cr0$	2	4.84	1.78	
119	$Cr0 \rightarrow O12 \rightarrow C10 \rightarrow C22 \rightarrow Cr0$	4	4.84	4.91	
120	$Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N2 \rightarrow Cr0$	4	4.85	4.62	
121	$Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$	4	4.85	2.89	
122	$Cr0 \rightarrow C7 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$	4	4.86	4.13	
123	$Cr0 \rightarrow C10 \rightarrow Cr0 \rightarrow N3 \rightarrow Cr0$	4	4.87	2.96	
124	$Cr0 \rightarrow C17 \rightarrow N1 \rightarrow N4 \rightarrow Cr0$	4	4.87	6.01	
125	$Cr0 \rightarrow C10 \rightarrow O12 \rightarrow N4 \rightarrow Cr0$	4	4.87	5.32	
126	$Cr0 \rightarrow C21 \rightarrow N1 \rightarrow C9 \rightarrow Cr0$	4	4.88	2.45	

127	$Cr0 \rightarrow C17 \rightarrow N2 \rightarrow N3 \rightarrow Cr0$	4	4.88	3.13
128	$Cr0 \rightarrow C22 \rightarrow C23 \rightarrow N3 \rightarrow Cr0$	4	4.90	4.91
129	Cr0→C7→N3→N3→Cr0	4	4.92	5.05
130	$Cr0 \rightarrow O12 \rightarrow C10 \rightarrow N4 \rightarrow Cr0$	4	4.92	5.70
131	$Cr0 \rightarrow C17 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	4	4.92	3.73
132	$Cr0 \rightarrow N4 \rightarrow C9 \rightarrow Cr0$	4	4.92	17.3
133	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C8 \rightarrow Cr0$	4	4.93	3.98
134	$Cr0 \rightarrow C22 \rightarrow Cr0 \rightarrow N1 \rightarrow Cr0$	4	4.93	5.92
135	$Cr0 \rightarrow N2 \rightarrow C22 \rightarrow N4 \rightarrow Cr0$	4	4.94	3.26
136	$Cr0 \rightarrow C10 \rightarrow N4 \rightarrow N3 \rightarrow Cr0$	4	4.95	4.81
137	$Cr0 \rightarrow C7 \rightarrow Cr0 \rightarrow N4 \rightarrow Cr0$	4	4.95	5.87
138	$Cr0 \rightarrow N1 \rightarrow Cr0 \rightarrow C10 \rightarrow Cr0$	4	4.95	19.8
139	$Cr0 \rightarrow C9 \rightarrow Cr0 \rightarrow N1 \rightarrow Cr0$	4	4.95	3.74
140	$Cr0 \rightarrow C13 \rightarrow C7 \rightarrow C8 \rightarrow Cr0$	4	4.95	5.51
141	$Cr0 \rightarrow C7 \rightarrow C13 \rightarrow N3 \rightarrow Cr0$	4	4.96	4.83
142	$Cr0 \rightarrow C8 \rightarrow N2 \rightarrow N1 \rightarrow Cr0$	4	4.96	3.70
143	$Cr0 \rightarrow C20 \rightarrow C17 \rightarrow Cr0$	4	4.97	1.45
144	$Cr0 \rightarrow N2 \rightarrow C7 \rightarrow C17 \rightarrow Cr0$	4	4.98	2.53
145	$Cr0 \rightarrow C18 \rightarrow C17 \rightarrow C9 \rightarrow Cr0$	4	4.98	4.71
146	$Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C9 \rightarrow Cr0$	4	4.98	3.12
147	Cr0→N1→C8→N3→Cr0	4	5.00	3.97
148	$Cr0 \rightarrow C21 \rightarrow Cr0 \rightarrow O5 \rightarrow Cr0$	4	5.00	1.60
149	$Cr0 \rightarrow C24 \rightarrow C22 \rightarrow Cr0$	4	5.01	8.95
150	$Cr0 \rightarrow N1 \rightarrow C20 \rightarrow C17 \rightarrow Cr0$	4	5.01	1.76
151	$Cr0 \rightarrow N2 \rightarrow C26 \rightarrow Cr0$	4	5.02	11.1
152	$Cr0 \rightarrow C17 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$	4	5.02	8.52
153	$Cr0 \rightarrow N1 \rightarrow C17 \rightarrow N4 \rightarrow Cr0$	4	5.05	2.90
154	$Cr0 \rightarrow N3 \rightarrow Cr0 \rightarrow C21 \rightarrow Cr0$	4	5.07	11.3
155	$Cr0 \rightarrow C22 \rightarrow N4 \rightarrow N2 \rightarrow Cr0$	4	5.08	1.94
156	$Cr0 \rightarrow C19 \rightarrow C21 \rightarrow Cr0$	4	5.11	6.25
157	$Cr0 \rightarrow C9 \rightarrow N2 \rightarrow N4 \rightarrow Cr0$	4	5.12	8.50
158	$Cr0 \rightarrow N4 \rightarrow C24 \rightarrow C26 \rightarrow Cr0$	4	5.12	6.03
159	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow N4 \rightarrow Cr0$	4	5.14	7.48
160	$Cr0 \rightarrow N1 \rightarrow C21 \rightarrow C18 \rightarrow Cr0$	4	5.15	4.40
161	$Cr0 \rightarrow C21 \rightarrow Cr0 \rightarrow N1 \rightarrow Cr0$	4	5.16	1.96
162	$Cr0 \rightarrow C19 \rightarrow C18 \rightarrow Cr0$	4	5.18	4.46
163	$Cr0 \rightarrow N4 \rightarrow C26 \rightarrow N2 \rightarrow Cr0$	4	5.18	7.33
164	$Cr0 \rightarrow C21 \rightarrow N1 \rightarrow N3 \rightarrow Cr0$	4	5.18	7.19
165	$Cr0 \rightarrow C22 \rightarrow N3 \rightarrow C22 \rightarrow Cr0$	2	5.19	0.86
166	$Cr0 \rightarrow C23 \rightarrow C24 \rightarrow N4 \rightarrow Cr0$	4	5.19	4.51
167	$Cr0 \rightarrow C8 \rightarrow C17 \rightarrow Cr0$	4	5.20	2.07
168	$Cr0 \rightarrow C24 \rightarrow C23 \rightarrow C22 \rightarrow Cr0$	4	5.20	5.68
169	$Cr0 \rightarrow N2 \rightarrow C7 \rightarrow O11 \rightarrow Cr0$	4	5.22	3.53

170	$Cr0 \rightarrow C15 \rightarrow Cr0$	2	5.23	9.74	
171	$Cr0 \rightarrow C17 \rightarrow C19 \rightarrow C17 \rightarrow Cr0$	2	5.24	1.96	
172	$Cr0 \rightarrow O5 \rightarrow N4 \rightarrow O5 \rightarrow Cr0$	2	5.25	3.08	
173	$Cr0 \rightarrow C20 \rightarrow C17 \rightarrow N1 \rightarrow Cr0$	4	5.25	2.01	
174	Cr0→C19→C20→Cr0	4	5.25	3.20	
175	$Cr0 \rightarrow C15 \rightarrow C8 \rightarrow Cr0$	4	5.25	17.0	
176	$Cr0 \rightarrow C8 \rightarrow N2 \rightarrow C8 \rightarrow Cr0$	2	5.26	2.47	
177	$Cr0 \rightarrow C20 \rightarrow C19 \rightarrow N1 \rightarrow Cr0$	4	5.26	3.12	
178	$Cr0 \rightarrow C7 \rightarrow C14 \rightarrow C7 \rightarrow Cr0$	2	5.27	6.50	
179	$Cr0 \rightarrow N2 \rightarrow C9 \rightarrow C13 \rightarrow Cr0$	4	5.29	4.51	
180	$Cr0 \rightarrow C24 \rightarrow C25 \rightarrow C26 \rightarrow Cr0$	4	5.30	3.19	
181	$Cr0 \rightarrow O12 \rightarrow N3 \rightarrow C10 \rightarrow Cr0$	4	5.32	7.62	
182	$Cr0 \rightarrow O12 \rightarrow C10 \rightarrow O12 \rightarrow Cr0$	2	5.32	6.31	
183	$Cr0 \rightarrow C23 \rightarrow N4 \rightarrow C22 \rightarrow Cr0$	4	5.39	4.92	
184	$Cr0 \rightarrow C14 \rightarrow C13 \rightarrow Cr0$	4	5.42	8.84	
185	$Cr0 \rightarrow N4 \rightarrow N1 \rightarrow C9 \rightarrow Cr0$	4	5.42	2.97	
186	$Cr0 \rightarrow C15 \rightarrow C16 \rightarrow Cr0$	4	5.44	8.74	
187	$Cr0 \rightarrow C15 \rightarrow C7 \rightarrow Cr0$	4	5.44	7.80	
188	$Cr0 \rightarrow C16 \rightarrow C15 \rightarrow C8 \rightarrow Cr0$	4	5.44	8.49	
189	$Cr0 \rightarrow C8 \rightarrow O5 \rightarrow N3 \rightarrow Cr0$	4	5.45	3.66	
190	$Cr0 \rightarrow C8 \rightarrow C14 \rightarrow C7 \rightarrow Cr0$	4	5.46	6.44	
191	$Cr0 \rightarrow C15 \rightarrow N3 \rightarrow Cr0$	4	5.47	7.14	
192	$Cr0 \rightarrow C9 \rightarrow C10 \rightarrow Cr0$	2	5.49	2.77	
193	$Cr0 \rightarrow C7 \rightarrow C14 \rightarrow N2 \rightarrow Cr0$	4	5.50	7.29	

^{*a*} The atom numbering scheme is shown in Figure 5.26. ^{*b*} R is the total distance travelled by the photoelectron divided by two. ^{*c*} The importance factor is the percent contribution of a path relative to the strongest MS path and includes Debye-Waller contributions.

atom	σ^2 (Å ²)	atom	σ^2 (Å ²)
N1	0.0010(1)	N2	0.0010(1)
O5	0.0020(7)	Cl6	0.0038(3)
C7	0.0020(1)	C9	0.0010(1)
O11	0.003(1)	C13	0.0030(1)
C14	0.0040(1)	C17	0.020(1)
C18	0.0020(1)	C19	0.0030(6)
C20	0.030(1)	C21	0.018(1)

Table S10. Debye-Waller factors for model **III** of $1.DMF.0.5H_2O^a$

^{*a*} The Monte-Carlo errors in the last significant figure are given in parentheses.



Figure S1. X-band EPR spectra of the Cr(V) products of the iodosobenzene oxidation of $1.H_2O$ in acetonitrile recorded at: (a) 5 min, (b) 10 min, (c) 20 min, (d) 30 min, (e) 60 min, and (f) 90 min after the addition of the oxidant.



Figure S2. X-band EPR spectra of the Cr(V) products obtained during the *tert*butylhydroperoxide oxidation of **1**.H₂O in acetonitrile recorded at: (a) 5 min, (b) 10 min, (c) 20 min, (d) 40 min, (e) 60 min, and (f) 90 min after the addition of the oxidant.



Figure S3 X-band EPR spectra of the Cr(V) products obtained during the iodosobenzene oxidation of **2** in DMF recorded at: (a) 5 min, (b) 10 min, (c) 20 min, (d) 40 min, (e) 60 min, and (f) 90 min after the addition of the oxidant. Parameters: receiver gain, 6.32×10^4 ; sweep width, 100 G; power, 20.17 mW; modulation amplitude, 1.00 G; scans, 3.



Figure S4 Low-temperature (~77 K) X-band EPR spectra of (a) Na[$Cr^{V}O(ehba)_{2}$] (10 mM in DMF) and (b) Oxidation of ~5 mg mL⁻¹ of **1**.H₂O with ~20 mg of PhIO in DMF reacted for 10 min at ~25 °C. Modulation amplitude, 5.0 G.



Figure S5 Observed EXAFS curves for $1.DMF.0.5H_2O$ (solid line) and 2 (dashed line) showing the effect of substitution of the Cl⁻ axial ligand by a H₂O ligand.