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THE STRUCTURE OF A NOVEL COMPLEX DERIVED FROM CYCLOOCTADIENETRICARBONYLRUTHENIUM*,**

F. A. COTTON*** and MARIE D. LaPRADE
Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 (*U.S.A.*)

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SUMMARY

When (1,5-cyclooctadiene)tricarbonylruthenium is treated first with $(C_6H_5)_3$-CBF_4 and then with sodium cyanide, a product of formula $(C_8H_{11}CN)Ru(CO)_3$ is isolated. In order to elucidate the chemistry of this and similar reactions, the structure of this substance has been determined by X-ray crystallography. It is found that the structure involves a cyanocyclooctadienyl ring bound to $Ru(CO)_3$ through a C–Ru σ bond and a *trihapto*-allyl group. The CN group is in an *exo* position. The systematic name of the compound is 1,2,3,6-*tetrahapto*-(5-cyanocyclooctadienyl)tricarbonylruthenium. The compound crystallizes in space group *Pbca* with unit cell dimensions $a = 22.756(14)$ Å, $b = 8.296(5)$ Å and $c = 13.186(12)$ Å. The observed density, 1.69(1) g/cm^3, agrees well with a calculated density of 1.698 for $Z = 8$; the molecule occupies a general position. Using 1373 statistically significant reflections collected on a counter diffractometer with Mo-K_α radiation, the structure was solved by Patterson and Fourier methods and refined to final residuals of $R_1 = 0.048$ and $R_2 = 0.047$. All hydrogen atoms were refined with isotropic temperature parameters, while all other atoms were assigned anisotropic temperature parameters.

INTRODUCTION

The treatment of (1,5-cyclooctadiene)$M(CO)_3$ compounds, M = Fe, Ru, Os, with the hydride abstracting reagent $(C_6H_5)_3CBF_4$ generates several types of cationic complexes, $[C_8H_{11}M(CO)_3]^+$, from which neutral molecules structurally different from the original 1,5-C_8H_{12} complexes can be obtained on treatment of these cations with nucleophiles.

In a previous communication[1] it was proposed that one important reaction sequence beginning with tricarbonyl(1,5-cyclooctadiene)metal(0) complexes is:

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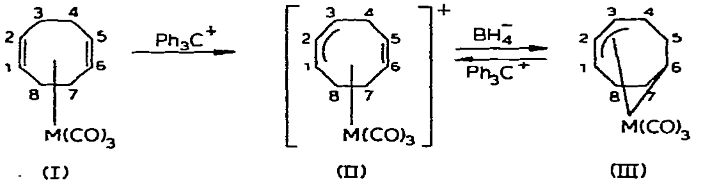
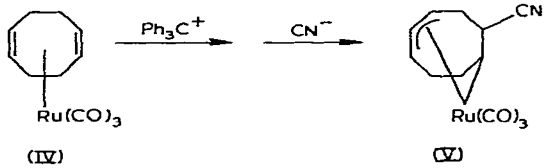
*** Address correspondence to this author at: Department of Chemistry, Texas A & M University, College Station, Texas 77843.



(1)

The use of nucleophiles, other than H^- (as BH_4^-), for example, CN^-, whose location in the products can be ascertained, is of interest because of the information thus provided about the detailed course of the reactions. We report here on one example, namely the transformation of (IV) into (V) and the characterization of the product (V). The structure confirms the general views which have been given[1] as to the course of this and related reactions.



PROCEDURE

The sample of $C_8H_{11}CNRu(CO)_3$ was supplied by Professor J. Lewis and Dr. B. F. G. Johnson. White single crystals suitable for X-ray work were obtained by crystallization from $CHCl_3$ and were mounted in thin-walled Lindeman glass capillaries. Single crystals examined by Weissenberg and precession photography were found to be orthorhombic. The systematic absence, $h0l$ for $l=2n+1$, $0kl$ for $k=2n+1$ and $hk0$ for $h=2n+1$, identified the space group as *Pbca* (no. 61). The unit cell dimensions at 24.8° are $a=22.756(14)$ Å, $b=8.296(5)$ Å, $c=13.186(12)$ Å. The quoted values for a, b and c were derived from a least-squares refinement of the setting angles for 26 manually centered reflections on a General Electric XRD-5 manual diffractometer using copper radiation, $\lambda(K_{\alpha 1})=1.5405$ Å; $\lambda(K_{\alpha 2})=1.5443$ Å.

The density was measured by flotation in aqueous barium iodide solution as 1.69 ± 0.01 g/cc. The density calculated from the formula weight of 318.296, the unit-cell volume of 2489.3 Å^3, and $Z=8$ is 1.698 g/cc. With $Z=8$ in the space group *Pbca* there are no crystallographic symmetry elements imposed on the molecule.

Intensities were measured using a crystal with approximate dimensions of $0.26\times0.20\times0.33$ mm; crystal faces were (011), (100), $(\bar{1}00)$, (001), $(00\bar{1})$, (101), $\bar{1}0\bar{1})$, $(0\bar{3}\bar{1})$ and $(02\bar{3})$. The crystal was aligned with its a^* axis coincident with the ϕ axis of the goniometer. Mo-K_α radiation $[\lambda(K_{\bar{\alpha}})=0.7107]$ filtered by zirconium foil was used to measure 1996 independent reflections (including 322 systematically absent in *Pbca*) within the sphere $\theta\leqslant25°$. Intensities were measured by a scintillation counter with the pulse-height discriminator set to accept 95% of the Mo-K_α peak. The distances from the crystal to the source and from the crystal to the circular screening aperture (2°) were 14.6 cm and 17.9 cm, respectively. A moving-crystal-moving-counter scan technique was employed with a scan range of 1.33° to conform with the mosaic spread of the crystal and a take-off angle of 2°. The scan rate was 4°/min.

The centering and intensity of five reflections (1200; 040, 925, 464, and 002) were checked every 100 reflections. They followed the same decay rate,which was linear with time of exposure of the crystal to the X-ray beam. At the completion of taking the data set this decrease was 19% of the original intensity. The integrated intensities were obtained from the total counts (P) of a coupled $2\theta-\omega$ scan from $2\theta_{\text{calcd.}}-0.66°$ to $2\theta_{\text{calcd.}}+0.67°$ and stationary background measurements (B_1, B_2) of 10 sec duration at the limits of each scan. Assuming that the background varies linearly (or gives an equivalent integrated total) through the scan range and taking the decomposition into account $I=(P-B_1-B_2)/(1-K\cdot t)$, where t = time of exposure (in min) and K is a constant derived from the above named five reflections by plotting $[I(t=0)-I(t)]/I(t=0)$ *versus* time and fitting a least-squares line. The standard deviation in the intensity was defined as

$$\sigma(I)=\left\{\frac{P+B_1+B_2+[0.02\cdot(P-B_1-B_2)]^2}{(1-K\cdot t)^2}+\left[\frac{(P-B_1-B_2)\cdot t\sigma(K)}{(1-K\cdot t)^2}\right]^2\right\}^{\frac{1}{2}}$$

In the latter stages of data collection eight reflections of $hk0$ for which $h=2n+1$ were found to have $I>3\sigma(I)$, the largest of which was 510 at $I=15\sigma(I)$, indicating that the space group might be $Pbcm$ or $Pbc2_1$.

As the intensities were converted to values of F_o^2 and F_o (on a relative scale) 631 reflections (including 86 reflections on $hk0$ for which $h=2n+1$ and 236 other systematic absences) were rejected using the criterion $I<2\sigma(I)$. Only the remaining 1373 reflections were used in solving and refining the structure. Of these 134 had $2<I/\sigma(I)\leqslant 3$, 271 had $3<I/\sigma(I)\leqslant 6$, 212 had $6<I/\sigma(I)\leqslant 10$ and 756 had $10<I/\sigma(I)\leqslant 50$. The data were corrected for absorption ($\mu=12.29$ cm^{-1}). The minimum and maximum transmission coefficients were 0.61688 and 0.76829. The average transmission coefficient was 0.66782. The R.M.S. variation in transmission coefficients was 0.02999 or 4.5%.

The Ru atoms were located in a three-dimensional Patterson map. Attempts to find the rest of the atoms using both Fourier and direct methods, assuming space group $Pbcm$, were unsuccessful. Using the space group $Pbc2_1$ and two independent molecules per unit cell, the remaining atoms (not including hydrogen atoms) were located. Refinement in $Pbc2_1$ by full-matrix, least-squares methods minimizing $\Sigma(|F_o|-|F_c|)^2$, converged at $R_1=\Sigma(||F_o|-|F_c||)/\Sigma|F_o|=0.065$. Scattering factors used here and subsequently were those of Cromer and Waber[2a]. Anomalous dispersion corrections[2b] for ruthenium, oxygen and nitrogen were included in the calculated structure factors. Weights were assigned using the relation $w=\sigma^{-2}$, where $\sigma=\sigma(I)/(2Lp\cdot F_o)$, with Lp representing the Lorentz and polarization corrections. Anisotropic temperature factors of the form $\exp[-(\beta_{11}\cdot h^2+\beta_{22}\cdot k^2+\beta_{33}\cdot l^2+2\beta_{12}\cdot h\cdot k+2\beta_{13}\cdot h\cdot l+2\beta_{23}\cdot k\cdot l)]$ were used for all atoms (except for hydrogen atoms introduced later).

At this point, the two independent molecules were found to be nearly in the relationship corresponding to an a glide plane perpendicular to the c axis. Many angles and distances which should have been chemically equivalent had widely disparate and relatively unreasonable values although averages of the pairs were quite acceptable. Refinement was therefore continued in space group $Pbca$ with one molecule in the asymmetric unit, and the eight nonzero reflections on $hk0$ with $h\neq 2n$ were deleted from the data set.

(continued on p. 351)

TABLE 1

THE OBSERVED AND CALCULATED STRUCTURE FACTORS

(× 10) (orbital *e*)

H	L	FOBS	FCAL
K = 0**			
4	0	4287	4357
8	0	1394	1457
10	0	413	427
12	0	1579	1635
14	0	559	619
16	0	1373	1396
20	0	656	653
24	0	457	442
0	2	1654	3325
1	2	1659	1486
3	2	1299	1171
4	2	3417	2584
5	2	1335	1259
6	2	1429	1319
7	2	1263	1101
8	2	3599	3397
10	2	276	270
12	2	1974	1574
14	2	212	139
15	2	245	248
16	2	1299	1743
18	2	111	113
19	2	204	219
20	2	595	577
21	2	219	214
24	2	413	372
0	4	1738	1619
1	4	1259	1205
2	4	946	906
3	4	1267	1159
4	4	3550	2953
5	4	94	104
6	4	249	271
7	4	543	571
8	4	2568	2554
9	4	764	729
10	4	449	437
11	4	444	452
12	4	1469	1461
13	4	1313	1048
16	4	897	972
17	4	276	273
19	4	301	308
20	4	524	506
21	4	149	159
24	4	299	299
0	6	2522	2282
1	6	715	718
2	6	362	333
3	6	917	905
4	6	1983	1910
5	6	1304	1326
6	6	447	449
7	6	551	561
8	6	1309	1311
9	6	587	582
10	6	154	147
11	6	285	311
12	6	1164	1180
13	6	357	371
14	6	288	303
15	6	157	217
16	6	541	512
17	6	293	288
18	6	133	139
19	6	264	288
20	6	361	340
21	6	272	263
22	6	109	67
23	6	136	109
24	6	199	186
0	8	566	555
1	8	756	746
2	8	334	349
3	8	853	838
4	8	825	838
5	8	711	732
7	8	870	871
8	8	736	719
9	8	642	648
11	8	477	473
12	8	749	735
13	8	283	282
15	8	332	323
16	8	333	334
17	8	338	337
19	8	129	168
20	8	325	307
21	8	248	270
0	10	408	393
1	10	663	669
3	10	572	574
4	10	614	630
5	10	449	452
7	10	464	459
8	10	403	386
9	10	672	689
11	10	334	331
12	10	165	174
13	10	359	358
15	10	445	450
16	10	231	229
17	10	232	242
19	10	224	242
20	10	175	185
0	12	293	279
1	12	551	548
2	12	168	126
3	12	424	433
4	12	249	254
5	12	518	513
6	12	199	191
7	12	515	519
8	12	215	204
9	12	476	459
11	12	392	392
13	12	265	286
15	12	293	292
17	12	204	159
1	14	347	382
3	14	369	349
5	14	375	354
7	14	366	384
9	14	257	252
11	14	333	289
K = 1**			
2	0	677	554
4	0	237	234
6	0	2713	1945
8	0	898	807
10	0	1191	1092
12	0	255	235
14	0	327	332
18	0	99	92
26	0	119	114
1	1	621	577
2	1	3735	3495
3	1	308	277
4	1	513	514
5	1	509	520
6	1	1451	1491
7	1	829	825
9	1	299	293
10	1	1651	1751
11	1	331	333
12	1	163	182
14	1	1179	1219
16	1	92	23
18	1	635	631
19	1	190	64
22	1	424	416
23	1	133	41
26	1	323	274
1	2	597	606
2	2	1338	1259
3	2	414	392
4	2	258	277
5	2	464	473
6	2	826	839
7	2	95	69
9	2	311	321
10	2	681	700
11	2	116	190
12	2	257	248
14	2	460	458
15	2	48	13
16	2	170	191
18	2	272	246
19	2	117	104
22	2	160	168
1	3	734	679
2	3	1639	1553
3	3	354	344
4	3	1379	1338
5	3	645	678
6	3	2137	2190
7	3	823	809
8	3	366	372
9	3	384	449
10	3	1400	1402
11	3	452	469
12	3	341	339
13	3	529	558
14	3	1121	1125
15	3	195	214
16	3	163	136
17	3	233	275
18	3	798	891
22	3	388	393
26	3	190	181
1	4	515	505
2	4	1257	1240
3	4	116	107
5	4	576	561
6	4	492	468
7	4	245	238
10	4	464	470
12	4	166	162
13	4	140	143
14	4	437	459
17	4	94	73
18	4	313	299
22	4	161	159
21	4	112	56
1	5	956	899
2	5	1848	1793
3	5	1017	987
5	5	997	962
6	5	1853	1833
7	5	824	828
9	5	485	514
10	5	1295	1285
11	5	462	470
13	5	426	444
14	5	847	857
15	5	307	336
17	5	396	415
18	5	409	417
19	5	211	242
20	5	112	130
21	5	152	172
22	5	293	292
23	5	171	132
2	6	978	964
3	6	181	143
4	6	183	160
6	6	818	816
7	6	116	116
8	6	290	281
10	6	376	359
12	6	114	66
14	6	244	254
15	6	187	191
1	7	911	899
2	7	1377	1354
3	7	439	432
4	7	362	359
5	7	1372	1356
6	7	771	909
7	7	448	461
9	7	873	867
10	7	467	934
11	7	493	486
12	7	38	190
13	7	194	214
14	7	727	717
15	7	244	250
16	7	139	115
17	7	212	224
18	7	335	319
19	7	265	272
21	7	139	167
22	7	241	219
23	7	129	107
1	9	908	979
2	9	742	787
3	9	638	644
4	9	732	757
6	9	703	717
7	9	485	506
8	9	93	43
9	9	501	502
10	9	436	425
11	9	429	456
12	9	190	181
13	9	401	398
14	9	319	299
15	9	296	288
17	9	358	355
18	9	338	324
19	9	266	266
21	9	158	156
22	9	131	169
1	8	265	248
2	8	313	318
3	8	141	146
4	8	152	165
5	8	322	335
6	8	377	364
9	8	90	82
10	8	336	331
11	8	143	127
14	8	305	298
15	8	110	111
18	8	131	171
1	10	121	130
2	10	277	308
5	10	295	205
6	10	225	207
7	10	150	128
9	10	140	159
10	10	233	232
11	10	223	227
13	10	114	108
14	10	123	148
15	10	214	182
17	10	129	97
18	10	116	91
1	11	598	615
2	11	405	418
3	11	541	538
4	11	187	183
5	11	491	500
6	11	477	494
7	11	508	531
8	11	110	133
9	11	352	382
10	11	266	269
11	11	450	451
13	11	374	377
14	11	120	110
15	11	287	245
17	11	303	295
18	11	150	134
19	11	166	154
1	12	251	264
2	12	162	149
3	12	276	256
5	12	138	157
6	12	238	188
7	12	210	217
9	12	124	111
10	12	132	78
11	12	126	116
1	13	358	362
2	13	149	120
3	13	457	448
5	13	429	434
6	13	112	124
7	13	434	432
9	13	426	433
10	13	106	96
12	13	299	266
13	13	292	266
1	14	157	148
3	14	131	142
5	14	165	161
7	14	160	134
9	14	127	138
1	15	289	292
3	15	316	307
5	15	242	254
7	15	242	230
K = 2**			
3	0	3514	3408
2	0	393	421
4	0	1297	1265
6	0	267	258
8	0	1354	1098
10	0	207	228
12	0	896	907
14	0	222	205
16	0	580	662
20	0	226	213
24	0	307	297
0	1	1417	1357
1	1	327	309
2	1	333	322
3	1	733	696
4	1	1298	1229
7	1	335	352
8	1	959	962
9	1	87	74
10	1	111	104
12	1	635	655
14	1	84	31
16	1	563	575
17	1	133	45
20	1	297	281
24	1	181	173
0	2	1399	1375
1	2	463	475
2	2	277	278
3	2	106	95
4	2	1178	1168
5	2	361	346
6	2	509	500
8	2	1533	1600
9	2	338	349
10	2	239	254
11	2	332	349
12	2	888	939
13	2	143	145
15	2	591	587
17	2	111	94
20	2	314	299
24	2	239	243
0	3	1229	1202
1	3	552	532
2	3	214	280
3	3	775	763
4	3	562	547
5	3	362	357
6	3	96	123
7	3	213	243
8	3	840	842
9	3	189	193
10	3	212	203
11	3	121	168
12	3	932	942
13	3	133	131
14	3	106	105
15	3	151	185
16	3	513	502
19	3	129	161
20	3	341	329
22	3	110	97
24	3	203	221
0	4	1394	1391
1	4	534	595
2	4	563	533
3	4	651	646
4	4	1671	1490
5	4	312	317
6	4	342	372
7	4	267	288
8	4	897	904
9	4	636	627
10	4	283	292
11	4	474	498
12	4	580	696
13	4	311	320
15	4	196	192
16	4	556	597
19	4	111	138
20	4	384	385
21	4	124	125
24	4	175	162
0	5	1305	1248
2	5	187	167
3	5	499	486
4	5	1264	1228
5	5	386	392
7	5	571	582
8	5	375	380
9	5	430	433
10	5	165	177
11	5	484	489
12	5	541	641
13	5	214	221
15	5	200	201
16	5	399	396
17	5	126	131
19	5	138	141
20	5	246	247
21	5	156	115
24	5	116	128
0	6	1236	1204
1	6	656	651
2	6	252	247
3	6	366	375
4	6	1125	1128
5	6	897	904
6	6	148	157
7	6	236	229
8	6	330	327
9	6	243	247
11	6	208	235
12	6	768	776
14	6	58	90
15	6	171	219
16	6	453	459
17	6	145	172
18	6	121	111
19	6	240	239
20	6	257	257
21	6	226	191
24	6	154	112
0	7	936	951
1	7	812	815
2	7	113	142
3	7	751	749
4	7	1064	1054
5	7	711	708
7	7	489	486
8	7	620	623
9	7	273	271
10	7	122	106
11	7	265	339
12	7	401	397
13	7	145	127
15	7	210	239
16	7	374	351
19	7	134	167
20	7	230	211
21	7	120	98
23	7	125	63
0	9	384	433
1	9	384	376
2	9	215	248
3	9	417	500
4	9	422	409
5	9	337	345
6	9	147	128
7	9	464	469
8	9	510	497
9	9	314	333
11	9	303	308
12	9	541	527
13	9	261	263
15	9	264	255
16	9	260	252
17	9	118	150
19	9	144	163
20	9	133	123
0	8	385	398
1	8	451	502
2	8	359	369
3	8	667	665
4	8	683	700
5	8	401	417
6	8	146	173
7	8	700	701
8	8	584	580
9	8	376	394
11	8	192	217
12	8	300	349
13	8	295	317
15	8	208	202
16	8	233	232
17	8	256	270
19	8	216	197
20	8	203	198
0	10	464	464
1	10	550	539
3	10	672	654
4	10	522	520
5	10	248	231
7	10	531	526
8	10	335	312
9	10	403	478
11	10	260	261
12	10	152	138
13	10	357	347
15	10	317	303
16	10	140	159
18	10	187	204
19	10	161	157
20	10	183	179
0	11	456	517
1	11	331	309
3	11	368	379
4	11	444	429
5	11	294	314
6	11	103	94
7	11	377	380
8	11	248	249
9	11	403	395
11	11	251	292
12	11	134	116
13	11	245	257
15	11	211	193
17	11	161	151
0	12	158	157
1	12	509	510
3	12	352	363
4	12	170	184
5	12	439	463
7	12	332	344
8	12	198	183
9	12	393	404
11	12	368	297
12	12	121	63
13	12	217	203
15	12	246	243
1	13	436	422
3	13	327	347
4	13	138	137
5	13	334	338
7	13	235	242
9	13	218	212
11	13	255	177
13	13	110	99
1	14	310	318
3	14	250	234
5	14	363	367
7	14	309	294
9	14	226	219
1	15	155	172
3	15	220	199
5	15	169	164
K = 3**			
2	0	2909	2837
4	0	92	61
6	0	2029	2044
8	0	300	297
10	0	1303	1353
14	0	949	949
18	0	626	678
22	0	315	289
1	1	684	657
2	1	1747	1287
3	1	214	213
4	1	295	288
5	1	167	151
6	1	676	704
7	1	216	237
8	1	155	209
9	1	126	126
10	1	393	436
11	1	156	183
14	1	527	544
18	1	305	278
22	1	181	153
1	2	900	877
2	2	2532	2493
3	2	225	221
5	2	394	371
6	2	1450	1459
8	2	72	57
10	2	1217	1241
11	2	279	285
12	2	95	74
14	2	961	972
15	2	205	196
16	2	86	84
17	2	111	153
18	2	585	583
22	2	363	345
24	2	100	25
1	3	75	62
2	3	1159	1180
4	3	309	319
6	3	790	818
7	3	196	209
8	3	132	116
10	3	614	645
11	3	89	107
12	3	301	306
13	3	149	159
14	3	377	386
18	3	243	253
22	3	174	189
1	4	358	358
2	4	1375	1361
3	4	328	324
4	4	186	182
5	4	333	332
6	4	1316	1339
7	4	352	380
8	4	99	119
9	4	221	217
10	4	1230	1239
11	4	260	272
12	4	101	88
13	4	188	224
14	4	784	796
15	4	242	254
17	4	228	254
18	4	398	398
19	4	203	208
21	4	124	165
22	4	255	267
23	4	116	101
1	5	335	353
2	5	552	547
4	5	141	124
6	5	759	770
7	5	144	163
9	5	108	130
10	5	655	674
11	5	99	195
13	5	128	124
14	5	386	428
18	5	198	205
19	5	109	94
22	5	125	126
1	6	425	412
2	6	1067	1042
3	6	436	451
4	6	265	271
5	6	718	696
6	6	1169	1176
7	6	598	615
9	6	563	549
10	6	718	731
11	6	457	469
13	6	251	253
14	6	405	401
15	6	302	307
17	6	113	151
18	6	277	277
19	6	164	193
21	6	132	121
22	6	177	200
23	6	132	75
1	7	127	127
2	7	577	590
4	7	319	317

(Table continued)

TABLE 1 (*continued*)

H	L	FOBS	FCAL
5	7	281	273
6	7	477	483
7	7	300	317
9	7	182	199
10	7	366	369
14	7	330	361
15	7	98	96
18	7	200	185
19	7	157	142
1	9	313	313
2	9	389	388
3	9	236	251
4	9	206	223
5	9	318	326
6	9	394	415
7	9	138	157
9	9	179	184
10	9	286	296
11	9	191	191
13	9	139	127
14	9	142	134
15	9	151	145
17	9	133	148
18	9	113	102
1	8	421	434
2	8	534	535
3	8	676	626
5	8	594	573
6	8	440	438
7	8	600	601
9	8	390	376
10	8	394	405
11	8	396	399
13	8	286	305
14	8	424	396
15	8	184	176
17	8	226	250
18	8	269	265
19	8	158	150
21	8	138	132
1	10	423	429
2	10	357	371
3	10	443	448
5	10	418	422
6	10	289	271
7	10	447	459
9	10	448	433
10	10	276	293
11	10	341	337
13	10	374	383
14	10	198	210
15	10	215	212
17	10	254	258
18	10	116	110
19	10	200	183
1	11	306	304
2	11	243	231
3	11	173	161
5	11	270	278
6	11	162	175
7	11	216	236
9	11	204	195
10	11	115	69
11	11	260	261
13	11	158	159
1	12	440	445
2	12	145	148
3	12	470	450
5	12	407	413
6	12	217	235
7	12	396	396
9	12	334	320
10	12	112	118
11	12	278	273
13	12	237	220
15	12	155	153
1	13	133	144
3	13	267	266
7	13	228	249
1	14	274	307
3	14	242	236
5	14	378	344
6	14	110	38
7	14	212	208
9	14	291	275
K 6			
0	0	628	633
4	0	140	130
6	0	271	274
10	0	169	144
12	0	152	137
14	0	147	160
16	0	305	295
20	0	103	76
0	1	2126	2210
1	1	363	331
2	1	196	215
3	1	499	499
4	1	1717	1765
6	1	152	151
8	1	1457	1509
9	1	278	294
12	1	1117	1150
13	1	165	177
16	1	768	743
20	1	458	420
24	1	286	262
0	2	787	773
1	2	123	105
4	2	297	315
5	2	239	249
7	2	96	75
8	2	179	192
9	2	89	53
10	2	113	114
13	2	151	145
16	2	111	107
0	3	1542	1705
1	3	600	602
3	3	592	582
4	3	1458	1507
5	3	457	475
6	3	172	163
7	3	239	213
8	3	1375	1275
9	3	319	337
12	3	1342	1050
13	3	189	195
15	3	245	240
16	3	705	714
17	3	111	109
19	3	105	145
20	3	403	384
21	3	130	125
24	3	243	238
0	4	137	106
1	4	136	165
3	4	314	316
4	4	166	164
5	4	86	93
6	4	108	91
8	4	363	345
12	4	251	257
13	4	97	71
0	5	1218	1248
1	5	345	339
3	5	580	544
4	5	1276	1334
5	5	672	684
6	5	97	74
7	5	820	818
8	5	1129	1153
9	5	378	410
10	5	104	68
11	5	456	453
12	5	757	748
13	5	299	313
15	5	183	192
16	5	473	465
17	5	220	240
19	5	153	158
20	5	292	304
21	5	142	142
0	6	137	124
2	6	113	[illegible]
3	6	230	216
4	6	160	173
6	6	223	229
7	6	180	185
8	6	204	214
12	6	191	206
13	6	100	42
17	6	94	86
21	6	118	50
0	7	1316	1042
1	7	506	610
2	7	85	16
3	7	741	728
4	7	920	914
5	7	635	651
7	7	523	519
8	7	507	615
9	7	515	525
11	7	302	306
12	7	676	474
13	7	317	325
14	7	99	108
15	7	210	230
16	7	369	374
17	7	173	184
19	7	181	175
20	7	247	262
21	7	143	137
0	9	505	536
1	9	538	514
2	9	145	151
3	9	562	560
4	9	488	483
5	9	430	419
6	9	131	139
7	9	379	378
8	9	406	399
9	9	432	394
11	9	341	338
12	9	415	390
13	9	276	244
15	9	314	312
16	9	245	235
17	9	195	188
19	9	193	188
0	8	115	132
4	8	212	230
5	8	136	133
7	8	121	128
19	8	105	44
0	10	168	182
1	10	137	137
2	10	97	98
3	10	97	83
4	10	123	96
0	11	238	254
1	11	382	377
3	11	392	406
4	11	318	327
5	11	362	360
7	11	399	415
8	11	273	276
9	11	314	313
11	11	261	279
12	11	147	131
13	11	215	225
15	11	197	157
3	12	109	35
13	12	124	50
1	13	255	327
3	13	307	299
5	13	309	294
7	13	275	266
8	13	119	107
9	13	226	237
K 7			
2	0	1456	1585
4	0	223	242
6	0	1208	1262
8	0	119	112
10	0	1074	1130
12	0	92	102
14	0	734	724
18	0	365	366
22	0	272	262
1	1	212	243
2	1	118	71
3	1	148	129
5	1	85	107
6	1	231	243
10	1	211	203
11	1	114	62
16	1	89	60
18	1	54	57
22	1	111	24
1	2	340	373
2	2	1293	1353
3	2	83	46
6	2	1218	1229
7	2	205	217
8	2	185	189
10	2	1015	1024
11	2	310	301
12	2	58	101
13	2	154	169
14	2	691	704
18	2	399	393
22	2	269	239
2	3	190	160
3	3	137	175
5	3	232	234
6	3	155	142
7	3	140	135
9	3	151	158
10	3	134	127
14	3	150	154
15	3	53	50
18	3	135	140
1	4	106	61
2	4	1260	1270
3	4	267	250
5	4	411	413
6	4	1053	1058
7	4	352	352
8	4	122	131
9	4	422	418
10	4	734	717
11	4	152	166
13	4	162	167
14	4	547	564
15	4	125	130
18	4	429	400
19	4	136	116
22	4	208	219
1	5	124	107
2	5	558	548
3	5	178	183
5	5	107	100
6	5	253	255
10	5	120	98
11	5	100	91
12	5	51	63
1	6	324	319
2	6	911	911
3	6	540	543
4	6	89	42
5	6	371	361
6	6	691	710
7	6	446	455
9	6	249	263
10	6	531	551
11	6	180	201
13	6	144	158
14	6	421	435
15	6	151	175
17	6	197	178
18	6	291	305
19	6	167	152
1	7	89	86
2	7	184	203
4	7	189	182
5	7	108	47
6	7	285	276
8	7	122	122
10	7	299	299
13	7	53	86
14	7	164	150
2	9	187	216
4	9	138	129
6	9	141	160
9	9	127	108
1	8	509	486
2	8	520	533
3	8	318	317
4	8	229	224
5	8	390	374
6	8	446	454
7	8	348	349
9	8	219	229
10	8	417	428
11	8	372	364
13	8	238	243
14	8	329	329
15	8	209	293
17	8	190	193
18	8	233	187
1	10	409	394
2	10	306	321
3	10	292	279
5	10	454	442
6	10	397	319
7	10	357	281
9	10	323	326
10	10	151	209
11	10	278	277
13	10	193	213
14	10	104	139
15	10	174	187
2	11	139	146
3	11	98	89
6	11	122	139
10	11	103	115
1	12	329	316
3	12	365	355
5	12	285	299
6	12	139	159
7	12	308	281
9	12	223	223
1	13	158	105
4	13	124	109
K 8			
0	0	741	775
3	0	98	9
4	0	741	749
8	0	459	489
12	0	311	319
16	0	253	263
20	0	196	149
0	1	738	732
3	1	148	165
4	1	444	636
8	1	564	635
9	1	197	200
12	1	541	564
13	1	115	155
16	1	297	303
20	1	171	172
0	2	591	611
1	2	172	163
3	2	113	109
4	2	550	559
5	2	102	46
6	2	113	106
8	2	438	458
10	2	104	93
11	2	115	129
12	2	382	394
16	2	270	272
20	2	179	148
0	3	904	905
1	3	124	85
2	3	121	109
3	3	251	258
4	3	704	720
7	3	149	152
8	3	453	450
10	3	144	136
11	3	97	103
12	3	373	371
13	3	117	113
16	3	351	346
17	3	122	52
20	3	210	209
0	4	522	533
1	4	89	63
3	4	95	102
4	4	479	492
5	4	131	107
6	4	99	91
8	4	421	439
12	4	271	286
13	4	129	77
16	4	128	148
17	4	104	81
20	4	125	124
0	5	564	526
1	5	316	322
3	5	239	231
4	5	578	555
5	5	370	376
7	5	259	251
8	5	504	510
11	5	134	144
12	5	145	151
15	5	114	110
16	5	249	239
17	5	194	113
19	5	116	115
0	6	420	436
1	6	138	108
3	6	111	109
4	6	385	402
5	6	122	104
7	6	92	85
8	6	320	315
9	6	177	166
12	6	239	199
16	6	149	141
0	7	375	378
1	7	221	217
3	7	293	290
4	7	365	371
5	7	271	272
7	7	258	247
8	7	373	395
9	7	296	303
11	7	179	168
12	7	349	358
13	7	189	188
15	7	141	129
16	7	203	195
0	9	379	372
1	9	259	281
3	9	355	335
4	9	327	323
5	9	228	239
7	9	289	273
8	9	216	213
9	9	268	267
11	9	260	236
12	9	188	176
13	9	176	175
0	9	226	229
1	8	131	120
4	8	206	192
5	8	211	216
7	8	160	114
8	8	193	191
9	8	132	130
11	8	130	147
12	8	160	184
16	8	153	138
0	10	139	141
1	10	133	128
3	10	171	124
4	10	134	144
5	10	167	163
7	10	130	139
8	10	125	164
9	10	110	109
11	10	147	134
12	10	128	125
1	11	287	288
3	11	258	287
4	11	177	164
5	11	245	271
7	11	249	263
8	11	166	160
9	11	208	199
1	12	155	149
3	12	206	197
5	12	132	104
K 9			
2	0	559	548
4	0	152	162
6	0	249	226
10	0	189	148
14	0	253	256
16	0	100	55
18	0	191	176
1	1	104	88
2	1	518	527
3	1	212	224
4	1	153	141
6	1	480	488
7	1	118	75
8	1	100	85
10	1	397	402
14	1	340	335
18	1	218	222
1	2	198	205
2	2	345	351
3	2	140	102
4	2	115	136
6	2	355	351
8	2	103	76
9	2	116	120
10	2	357	346
14	2	240	241
17	2	132	100
18	2	128	122
1	3	210	209
2	3	421	430
3	3	194	185
4	3	118	119
5	3	193	209
6	3	440	462
7	3	121	103
8	3	117	87
9	3	157	153
10	3	434	424
14	3	262	266
18	3	149	164
1	4	166	114
2	4	375	369
5	4	283	276
6	4	358	359
8	4	196	172
10	4	282	272
11	4	125	103
14	4	166	152
16	4	107	32
1	5	288	285
2	5	454	466
3	5	146	158
4	5	94	2
5	5	286	272
6	5	371	366
7	5	173	165
9	5	224	237
10	5	261	262
11	5	158	162
13	5	181	167
14	5	199	198
15	5	100	70
2	6	301	284
3	6	206	206
5	6	107	115
6	6	277	259
7	6	194	181
10	6	216	215
11	6	94	54
14	6	176	171
1	7	222	208
2	7	323	311
3	7	276	269
5	7	224	199
6	7	257	244
7	7	257	261
9	7	219	190
10	7	181	178
11	7	199	182
13	7	108	143
14	7	191	173
1	9	219	189
2	9	226	209
3	9	246	219
5	9	219	210
6	9	177	167
7	9	183	170
9	9	186	183
10	9	153	145
11	9	149	108
1	8	133	126
2	8	207	230
3	8	149	121
5	8	165	131
6	8	204	209
7	8	149	150
9	8	141	128
10	8	191	188
13	8	126	117
1	10	171	152
2	10	160	143
3	10	149	147
5	10	183	156
7	10	157	144
1	11	235	230
2	11	107	89
K 10			
0	0	445	440
4	0	528	530
8	0	558	542
12	0	433	404
0	1	310	265
4	1	258	236
8	1	224	188
12	1	162	153
0	2	572	579
1	2	111	57
4	2	525	520
7	2	137	90
8	2	425	433
9	2	129	98
10	2	125	78
12	2	343	339
0	3	264	227
4	3	195	180
5	3	111	25
8	3	173	159
10	3	109	9
12	3	189	127
0	4	490	505
1	4	205	182
3	4	188	155
4	4	461	448
5	4	156	128
6	4	101	66
7	4	122	125
8	4	363	354
9	4	130	69
11	4	120	128
12	4	283	265
0	5	125	91
4	5	138	121
8	5	147	125
9	5	106	72
11	5	116	17
0	6	379	360
1	6	172	156
3	6	181	157
4	6	324	325
5	6	274	274
7	6	152	139
8	6	271	240
9	6	184	184
11	6	126	114
12	6	183	193
0	7	132	82
5	7	106	27
1	9	126	71
3	8	264	220
1	8	186	156
3	8	129	133
4	8	174	179
5	8	198	193
K 11			
2	1	386	392
5	1	348	344
10	1	294	297
1	3	129	90
2	3	347	361
5	3	163	98
6	3	348	334
7	4	100	58
1	5	141	109
2	5	336	317
5	5	117	104
6	5	270	251
1	6	110	33

TABLE 2

ATOMIC PARAMETERS

Atom	*Positional parameters*			*Thermal parameters* ($Å^2$)[a]						
	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}	B
Ru	0.62436(4)	0.55681(8)	0.26654(4)	5.72(3)	4.98(3)	3.65(3)	−0.26(5)	0.25(3)	−0.18(3)	
C'(1)	0.6198(5)	0.7867(11)	0.2311(6)	8.9(6)	4.8(4)	5.6(4)	−0.4(6)	−0.2(5)	−0.1(3)	
O(1)	0.6145(4)	0.9142(9)	0.2019(6)	14.2(7)	6.0(4)	8.1(4)	−0.7(5)	−1.7(4)	1.1(3)	
C'(2)	0.7033(4)	0.5341(14)	0.2100(6)	5.6(4)	9.7(7)	4.1(4)	−0.7(5)	−0.2(3)	1.7(4)	
O(2)	0.7475(4)	0.5160(14)	0.1806(5)	6.3(4)	20.6(1.0)	7.7(3)	−0.0(5)	2.4(4)	2.6(5)	
C'(3)	0.5798(4)	0.4955(1)	0.1506(6)	7.4(5)	5.6(5)	4.3(4)	1.1(4)	−0.3(4)	−0.1(3)	
O(3)	0.5508(3)	0.4525(10)	0.0858(5)	9.7(5)	10.9(5)	6.5(3)	1.4(5)	−2.7(3)	−2.6(4)	
C(1)	0.5493(5)	0.5387(14)	0.3774(7)	6.3(6)	6.7(6)	5.6(4)	1.7(5)	0.7(4)	−0.1(4)	
C(2)	0.5957(7)	0.6278(12)	0.4203(6)	8.6(6)	5.1(5)	3.9(3)	0.2(5)	1.4(4)	−1.0(3)	
C(3)	0.6533(5)	0.5670(13)	0.4322(6)	8.5(6)	5.7(5)	4.1(3)	−1.3(6)	−0.4(4)	−0.9(4)	
C(4)	0.6685(5)	0.3990(12)	0.4701(6)	6.2(6)	6.4(6)	4.5(4)	−0.3(4)	−0.7(4)	−0.3(3)	
C(5)	0.6769(4)	0.2792(11)	0.3830(6)	6.0(5)	5.6(5)	4.7(4)	−0.2(4)	0.1(4)	0.1(3)	
C(6)	0.6297(5)	0.3031(10)	0.3023(6)	5.4(4)	5.3(4)	4.1(3)	0.5(4)	0.3(3)	−0.5(3)	
C(7)	0.5677(4)	0.2422(13)	0.3324(8)	5.4(5)	5.9(5)	6.3(5)	−0.8(5)	−0.6(4)	0.2(4)	
C(8)	0.5356(5)	0.3606(15)	0.4005(9)	6.5(6)	8.1(7)	6.5(6)	1.8(5)	1.3(5)	0.3(5)	
C(9)	0.6796(5)	0.1106(13)	0.4199(7)	6.8(6)	6.6(6)	5.6(4)	0.5(5)	−0.3(4)	−0.5(4)	
N	0.6806(4)	−0.0208(11)	0.4471(7)	9.5(6)	5.7(5)	8.9(5)	0.7(5)	−0.7(4)	1.3(4)	
H(1)	0.518(3)	0.596(9)	0.365(5)							4.6(1.6)
H(2)	0.597(3)	0.750(9)	0.424(5)							5.0(1.4)
H(3)	0.682(3)	0.653(9)	0.452(5)							5.3(1.5)
H(41)	0.631(4)	0.358(12)	0.505(6)							7.6(2.2)
H(42)	0.704(4)	0.404(11)	0.501(7)							7.4(2.3)
H(5)	0.710(3)	0.307(9)	0.347(5)							4.6(1.5)
H(6)	0.634(3)	0.248(8)	0.253(5)							4.0(1.5)
H(71)	0.565(4)	0.136(11)	0.368(6)							6.3(2.0)
H(72)	0.540(4)	0.230(12)	0.275(7)							8.2(2.3)
H(81)	0.548(4)	0.340(13)	0.459(7)							7.4(2.6)
H(82)	0.488(5)	0.368(12)	0.396(7)							8.6(2.4)

[a] The B_{ij}'s, in $Å^2$, are related to the dimensionless β_{ij}'s employed during refinement as $B_{ij}=4\,\beta_{ij}/(a_i \cdot a_j^*)$.

After several cycles, with $R_1 = 0.057$ and $R_2 = \{w \cdot [|F_o| - |F_c|]^2 / \Sigma(w \cdot F_o^2)\}^{\frac{1}{2}} = 0.059$ an electron density difference map was computed and all of the hydrogen atoms were unambiguously located. The hydrogen atoms were refined isotropically while refinement of the other atoms was continued anisotropically. The refinement was considered complete when in one cycle no thermal or positional parameter changed by as much as 1/5 its estimated standard deviation. After this cycle R_1 was 0.048 and R_2 was 0.047. No systematic dependence of $w \cdot (F_o - F_c)^2$ on $|F_o|$ or $\sin \theta/\lambda$ was observed. In the final electron-density map the standard deviation in the electron density was 0.10 e/Å^3. The highest peak in the difference map was in the vicinity of the Ru atom and contained 0.97 e/Å^3. The final standard deviation of an observation of unit weight was 0.92. Of the 309 F_c values corresponding to reflections not included in the refinement, 106 were found to lie between $1.0 \times F_{\text{min}}$ and $1.5 \times F_{\text{min}}$, where F_{min} is the smallest F_{obs} included in the refinement, and one was between $1.5 \times F_{\text{min}}$ and $2.0 \times F_{\text{min}}$; none was higher than $2.0 \times F_{\text{min}}$.

Since refinement in *Pbca* was successful (lower *R* than in $Pbc2_1$ with half as many parameters) and since those reflections which violate the condition for the *a* glide did not change in intensity when the a^* axis was inclined at an angle of 18° with respect to the ϕ axis of the goniometer and are, therefore, not Renninger reflections, the appearance of the anomalous *hk*0 reflections is unexplained. A list of the F_o and final F_c values, in 0.1 electrons, is presented in Table 1.

The following computer programs were used: PICK2, J. A. Ibers, diffractometer settings; DR69, M. D. LaPrade, data reduction; DRAB70, B. G. DeBoer, absorption correction; FORDAP, A. Zalkin, Fourier syntheses; SFIX, local version of SFLS5, C. T. Prewitt, full-matrix least-squares refinement; MGEOM, J. S. Wood, least-squares planes; STAN1, B. G. DeBoer, distances, angles and e.s.d.'s; ORTEP,

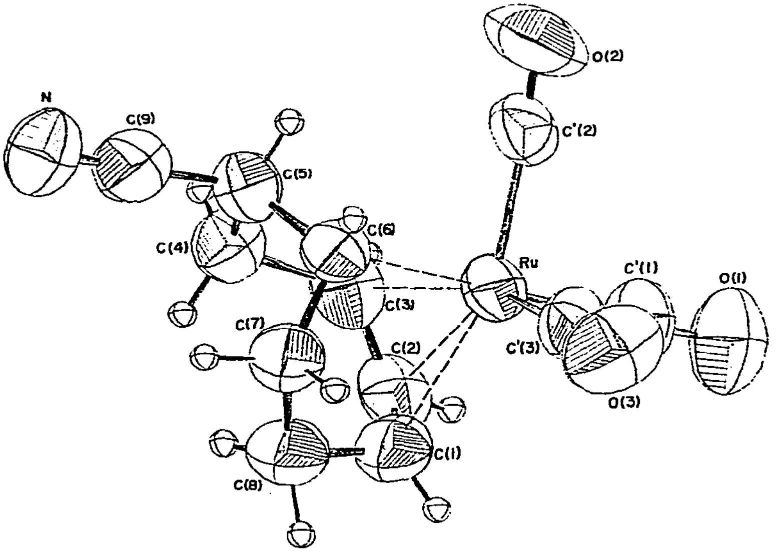


Fig. 1. A perspective view of the 1,2,3,6-*tetrahapto*-(5-cyanocyclooctadienyl)tricarbonyl ruthenium molecule showing ellipsoids of thermal motion which have been scaled to 50% probability distributions.

TABLE 3

BOND LENGTHS (Å)

Ru–C(1)	2.252(10)	C′(1)–O(1)	1.13(1)
Ru–C(2)	2.210(8)	C′(2)–O(2)	1.09(1)
Ru–C(3)	2.284(8)	C′(3)–O(3)	1.14(1)
Ru–C(6)	2.161(9)		
Ru–C′(1)	1.966(9)	C(1)–H(1)	0.88(7)
Ru–C′(2)	1.954(10)	C(2)–H(2)	1.02(8)
Ru–C′(3)	1.904(9)	C(3)–H(3)	1.00(8)
		C(4)–H(41)	1.02(10)
C(1)–C(2)	1.41(2)	C(4)–H(42)	0.91(10)
C(2)–C(3)	1.41(1)	C(5)–H(5)	0.92(7)
C(3)–C(4)	1.52(1)	C(6)–H(6)	0.80(6)
C(4)–C(5)	1.53(1)	C(7)–H(7)	0.99(8)
C(5)–C(6)	1.53(1)	C(7)–H(72)	0.99(9)
C(6)–C(7)	1.55(1)	C(8)–H(81)	0.84(9)
C(7)–C(8)	1.52(2)	C(8)–H(82)	1.09(10)
C(8)–C(1)	1.54(2)		
C(5)–C(9)	1.48(1)		
C(9)–N	1.15(1)		

TABLE 4

INTERATOMIC ANGLES (°)

C′(1)–Ru–C′(2)	93.0(5)	C(8)–C(1)–H(1)	113(5)
C′(1)–Ru–C′(3)	92.3(4)	C(2)–C(1)–H(1)	114(5)
C′(2)–Ru–C′(3)	99.0(4)	C(1)–C(2)–H(2)	124(4)
		C(3)–C(2)–H(2)	109(4)
Ru–C′(1)–O(1)	173.0(9)	C(2)–C(3)–H(3)	112(4)
Ru–C′(2)–O(2)	177.2(12)	C(4)–C(3)–H(3)	115(4)
Ru–C′(3)–O(3)	175.1(9)	C(3)–C(4)–H(41)	105(6)
		C(3)–C(4)–H(42)	108(6)
C(1)–C(2)–C(3)	123.6(10)	C(5)–C(4)–H(41)	103(5)
C(2)–C(3)–C(4)	125.0(10)	C(5)–C(4)–H(42)	105(6)
C(3)–C(4)–C(5)	112.2(7)	C(4)–C(5)–C(9)	111.8(7)
C(4)–C(5)–C(6)	110.6(8)	C(4)–C(5)–H(5)	109(5)
C(5)–C(6)–C(7)	114.8(7)	C(6)–C(5)–C(9)	112.4(8)
C(6)–C(7)–C(8)	112.3(9)	C(6)–C(5)–H(5)	100(5)
C(7)–C(8)–C(1)	113.9(9)	C(5)–C(6)–H(6)	113(5)
C(8)–C(1)–C(2)	125.2(10)	C(7)–C(6)–H(6)	98(5)
C(5)–C(9)–N	178.4(9)	C(6)–C(7)–H(71)	117(5)
		C(6)–C(7)–H(72)	115(6)
H(41)–C(4)–H(42)	104(8)	C(8)–C(7)–H(71)	106(5)
H(71)–C(7)–H(72)	103(8)	C(8)–C(7)–H(72)	102(6)
H(81)–C(8)–H(82)	114(9)	C(7)–C(8)–H(81)	104(7)
C(9)–C(5)–H(5)	112(5)	C(7)–C(8)–H(82)	119(5)
		C(1)–C(8)–H(81)	108(8)
		C(1)–C(8)–H(82)	98(5)

TABLE 5

MOLECULAR PLANES

1. Plane *A* containing C(1), C(2), C(3)
$-0.242\,x-0.349\,y+0.905\,z+0.080=0$
Distance of atoms from plane (Å)

H(1)	−0.14
H(2)	−0.32
H(3)	−0.17

2. Plane *B* containing C(1), C(3), C(4), C(8)
$-0.305\,x+0.254\,y+0.918\,z-1.887=0$
Distance of atoms from plane (Å)

C(1)	−0.0006	H(3)	0.22
C(3)	0.0006	H(41)	0.59
C(4)	−0.0004	H(42)	0.13
C(8)	0.0004	H(81)	0.57
H(1)	0.19	H(82)	0.29

3. Plane *C* containing C(4), C(5), C(7), C(8)
$-0.109\,x-0.739\,y+0.665\,z-0.001=0$
Distance of atoms from plane (Å)

C(4)	0.023	H(41)	0.68
C(5)	−0.028	H(42)	0.17
C(7)	0.029	H(71)	1.01
C(8)	−0.023	H(72)	−0.33
C(9)	1.324	H(81)	0.60
H(5)	−0.59	H(82)	0.00

4. Plane *D* containing C(5), C(6), C(7)
$-0.215\,x+0.898\,y+0.383\,z+0.702=0$
Distance of atoms from plane (Å)

C(9)	−1.084	H(71)	−0.61
H(5)	−0.15	H(72)	−0.23
H(6)	−0.69		

Angle between *A* and B 144°44′
Angle between *B* and C 117°6′
Angle between *C* and *D* 112°41′

C. K. Johnson, thermal ellipsoid drawings; PUBTAB, R. C. Elder, structure factor table.

RESULTS

The molecular structure and atom numbering scheme are shown in Fig. 1. The atomic positional and thermal parameters are presented in Table 2. The bond distances are given in Table 3 and various interatomic angles are listed in Table 4. Table 5 gives the equations for several planes, the distances of atoms from these planes and dihedral angles. In all tables, figures in parentheses are estimated standard deviations occurring in the least significant digit of the parameter.

DISCUSSION

The results presented here support the general scheme in eqn. (1) and, specifically, substantiate the correctness of structures of type (III). The location of the cyano group in (V) implies that this nucleophile attacks the intermediate, (II), from the *exo* direction at ring carbon atom 5. There is, of course, no certainty that all other nucleophiles, especially one as unique as H^-, do the same, but it seems likely that most of them will behave in the same way.

The carbocyclic ligand is attached to the ruthenium atom by a σ bond (2.16 Å) from C(6) and by coordination of a π-allyl group formed by C(1), C(2) and C(3) [Ru–C(1), 2.25 Å; Ru–C(2), 2.21 Å; Ru–C(3), 2.28 Å]. The cyano group occupies the *exo* position on C(5). The manner of attachment of the ring to the metal naturally requires extensive folding of the ring, and this can be seen in Fig. 1. All bond lengths within the ring system have reasonable values, *viz.*, C(5)–C(9), 1.48 Å; C(9)–N, 1.15 Å; C–C single bonds, 1.52–1.55 Å; C–C bonds in the π-allyl group, 1.41 Å. The Ru–C–O groups have Ru–C(av.) = 1.94 Å and C–O(av.) = 1.12 Å. The C–Ru–C angles average 94.8°.

The (π-allyl)–Ru bonding is generally typical of (π-allyl)–metal bonding in comparable systems. For example, in the molecules[3] $(h^5\text{-}C_5H_5)(CO)_2Mo(C_7H_7)$ and $(h^5\text{-}C_5H_5)(CO)_2Mo(C_7H_7)Fe(CO)_3$, the C_7H_7 rings are bound to the molybdenum atom through π-allyl moieties and the outer M–C distances exceed the inner M–C distances while the C–C distances are $\approx$1.41 Å. The $Ru(CO)_3$ group is not greatly different from that in $C_8H_8Ru(CO)_3$, where the mean Ru–C and C–O distances are 1.92 and 1.13 Å, respectively[4].

As often happens when seven- or eight-membered carbocyclic rings have a multiple attachment to a single metal atom, all C–C–C angles within the ring are greater than the ideal values for sp^2 or sp^3 hybridization. In this molecule, the former average 124.6 and the latter range from 110.6° to 114.7°. The C–C–H angles are correspondingly smaller.

The only previous indication that a cyclooctapolyene ring can bond to a metal in this 1,2,3,6-*tetrahapto* fashion is found in a cyclooctatetraene complex of tricarbonylosmium, where such a structure has been inferred from the ^1H NMR spectrum[5]. With the COT compound the 1,2,3,6-*tetrahapto* structure rearranges thermally to a 1,2,3,4-*tetrahapto* one, whereas, with 1,5-cyclooctadiene the 1,2,3,6-*tetrahapto* structure appears to be thermodynamically favored over the 1,2,5,6- or 1,2,3,4-*tetrahapto* ones[1].

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