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CRYSTAL AND MOLECULAR STRUCTURE OF (DITHIOFORMATO)BIS(TRIPHENYLPHOSPHINE)DICARBONYLRHENIUM, $Re(HCS_2)(CO)_2[P(C_6H_5)_3]_2$

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SUMMARY

The addition of CS_2 to hydridotris(triphenylphosphine)dicarbonylrhenium results in the formation of (dithioformato)bis(triphenylphosphine)dicarbonylrhenium. This complex crystallizes in the triclinic space group $P\bar{1}$; the reduced cell has dimensions: a 10.481(15) Å, $b=12.471(15)$ Å, $c=14.878(15)$ Å, $\alpha=81.78(7)°$, $\beta=74.03(7)°$, $\gamma=107.37(7)°$, $V=1735$ Å^3. The observed density is 1.63(2) g/cm^3 while the computed density for $Z=2$ is 1.615 g/cm^3. Intensities of 2682 independent reflections, having $\sigma(I)/I<0.25$, were measured by counter methods using a molybdenum source and a silicon monochromator. The structure was refined by full matrix least squares to a final R factor of 0.039. The crystal consists of a packing of discrete monomeric molecules; the distorted octahedral coordination around the metal atom has approximately a C_{2v} symmetry. The dithioformate anion chelates on rhenium atom with bonding parameters Re–S 2.500(3) Å and 2.532(5) Å, C–S 1.64(2) Å and 1.68(2) Å and S–C–S 116.7(1)°. The mean length of the two Re–P bonds is 2.42 Å and that of the two Re–C bonds is 1.91 Å. The Re–C–O interactions appear to be disordered and so does the chelate anion. On the basis of the present determination probable structures are suggested for other addition products formed from CS_2 and Rh^{III} and Ir^{I}complexes.

INTRODUCTION

A series of novel reactions based on addition of carbon disulphide to hydrido, alkyl and aryl complexes of rhodium, iridium and platinum has been recently reported by Wilkinson and coworkers[1]. Typical examples are the reaction of $IrH(CO)_2[P(C_6H_5)_3]_3$ to give $Ir(CO)(CS_2H)[P(C_6H_5)_3]_2$ and the reaction of $RhI_2(CH_3)[P(C_6H_5)_3]_3$ to give $RhI_2(CS_2CH_3)[P(C_6H_5)_3]_2$. Freni *et al.*[2] found that $ReH(CO)_2[P(C_6H_5)_3]_3$ reacts with CS_2 to give the diamagnetic complex $Re(CO)_2(CS_2H)[P(C_6H_5)_3]_2$, complete reaction occurring when the hydrido complex is allowed to react for one hour in boiling CS_2.

IR and NMR spectra do not answer the question of whether the insertion of CS_2 in metal hydrides results in the formation of dithioformato complexes $ML_n(HCS_2)$ or dithio acids ML_n (CSSH); equally uncertain is whether complexes of dithioanions $ML_n(RCS_2)$ or dithioesters $ML_n(CSSR)$ result when the parent complexes are alkyl or aryl derivatives[1,2]. The oxygen analogs of all these possible products are fairly well known. A formato complex has been described recently[3], which results from the insertion of CO_2 in $CoH(N_2)[P(C_6H_5)_3]_3$, and it has been demonstrated[4] that the unstable intermediate in the formation of hydrides from cationic carbonyl complexes possesses a carboxylic group bonded to the metal. On the other hand, carboalkoxy derivatives of, say, iridium are well characterized compounds[5], and so are the complexes of carboxylate anions.

The determination of the crystal structure of $Re(CO)_2(HCS_2)[P(C_6H_5)_3]_2$ was undertaken in order to solve the problem of whether acids or dithioformato complexes result upon insertion of CS_2 in the isoelectronic Re^I and Rh^{III} hydrides. When we began this determination, no structural reports had appeared on Re–S interactions nor on carbonylphosphine complexes of this metal; another aim of this work was, therefore, to gain some knowledge of these structural aspects of rhenium chemistry.

EXPERIMENTAL

Crystal data

$Re(CO)_2(HCS_2)[P(C_6H_5)_3]_2$, $M=842.2$, gives yellow crystals of an oblique prismatic habit. The *reduced* cell has the following dimensions $a=10.481\ (15)$ Å, $b=12.471\ (15)$ Å, $c=14.878\ (15)$ Å, $\alpha=81.78\ (7)°$, $\beta=74.03\ (7)°$, $\gamma=107.37\ (7)°$, $V=1735$ Å^3, space group $P\bar{1}$, C_i^1 (No. 2), $D_{meas.}=1.63(2)\ g\cdot cm^{-3}$ (by flotation in iodomercurate), $D_{calc.}=1.613\ g\cdot cm^{-3}$, $Z=2$.

The cell dimensions obtained from precession photographs were refined with the "ω-lag" method[6] on the Pailred diffractometer with Mo-$K\alpha_1$ radiation ($\lambda=0.70930$).

Intensity measurements

The crystal used in the collection of intensities was an oblique parallelopiped having dimensions, in mm, of $0.05\times0.10\times0.26$, mounted along the c axis—the direction of maximum elongation—on the linear equi-inclination Pailred diffractometer. The incident radiation was the Mo-$K\alpha$ doublet, obtained by monochromatisation of the primary beam on a silicon single crystal. The intensities were measured within the limit of $2\theta=47°$, using the ω scan technique at a rate of 0.5°/min; the scan interval for each reflection varied from 1° to 2° depending upon the equi-inclination angle. The backgrounds were measured for one minute at the lower and upper limits of the scanning range.

The crystal reflecting power was monitored by measuring a small set of standard reflections during the data collection; no decay was apparent, so all the intensities belonging to the various levels of the reciprocal lattice (from $hk0$ to $hk11$) were given the same scale factor throughout the refinement. The integrated intensities were then corrected for Lorentz, polarisation and absorption effects ($\mu=39.9\ cm^{-1}$). The transmission factors, computed with the Busing and Levy routine[7] with a point sampling $6\times6\times6\ (=216)$, were in the range 0.69–0.83. The polarisation correction was applied, taking account of the partial polarisation of the incident monochromatized beam[8].

From all the observed intensities a final set of 2682 independent F_o's was gathered, corresponding to all observations measured with a relative counting statistical error, $\sigma(I)/I$, less than 0.25*.

Determination and refinement of the structure

The structure was solved by the conventional Patterson and Fourier techniques. After location and preliminary refinement of the co-ordinates of the rhenium atom, a difference Fourier synthesis allowed the positions of all non hydrogen atoms to be recovered. The conventional R factor, based upon the contribution of all these atoms was 0.13.

The least squares refinement was carried out in two steps. In the first (a block refinement), the Re atom was treated anisotropically and all the remaining atoms isotropically; the phenyl rings were treated as rigid C_6 groups of D_{6h} symmetry, with a C–C bond length of 1.395 Å. In a Fourier difference computed at the end of this stage ($R=0.072$), all the hydrogen atoms of the phenyl rings appeared in their expected positions. The second stage of refinement, by full matrix least squares, included the anisotropic thermal parameters of all the non-group atoms; the groups were treated as rigid C_6H_5 rings, each one with a mean isotropic thermal factor. This second stage converged to the following reliability indices: $R=\Sigma(||F_o|-|F_c||)/\Sigma|F_o|=0.039$ and $R_w=(\Sigma w(|F_o|-|F_c|)^2/\Sigma w\cdot|F_o|^2)^{\frac{1}{2}}=0.049$. The weighting scheme adopted is given by the expression: $w=1/(7+10^{-2}\times|F_o|+5\times10^{-4}\times|F_o|^2)$; the coefficients in the polynomial were chosen in order to obtain an approximately constant value of the mean $(w\cdot\Delta F^2)$ over the entire range of F and of $\sin\theta/\lambda$.

The structure factor and least squares computations were based upon the atomic scattering factors of Cromer and Mann for Re, S, P, and C atoms[9]; the hydrogen scattering factor was that given by Forsyth and Wells[10]. The real and imaginary contribution. All the remaining signals were in the range ±0.3 $e^-/\text{Å}^3$; no putations[11].

A final Fourier difference revealed one signal of about 1.5 electrons per Å^3 in the position of the Re atom. This was probably due to the combined effect of possible inaccuracy in the tabulated corrections for anomalous dispersion and to the fact that the Fourier summation—a complex function when anomalous scatterers are involved, even if the space group has centres of symmetry—did not include the imaginary contribution. All the remaining signals were in the range — ±0.3 $e^-/\text{Å}^3$; no signals were obtained corresponding to the presence of an hydrogen atom associated with the metal atom nor with the CS_2 group.

Computations

All the computations described in this paper were carried out on an IBM 7040 computer. Counter data reduction, absorption correction and statistical analysis for weighting schemes were based upon Fortran programs written in the Authors' laboratory. For Fourier analyses, structure factors and least squares, local versions were used of the following entries in the 1966 "International World List of Crystallographic Programs": 7528, 7531, 7532 and 7535; a program written by Domenicano and Vaciago of the University of Rome was used in the computation of the molecular parameters.

(*continued on p.* 81)

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* The counting statistical esd. of the net intensity I is equal to $(I_{\text{peak}}+t^2\cdot I_{\text{background}})^{\frac{1}{2}}$, t being the ratio between times spent on peak and background measurement.

TABLE I

STRUCTURE FACTOR MODULI IN ELECTRONS FOR $Re(HCS_2)(CO)_2[P(C_6H_5)_3]_2$

H	L	FO	/FC/
K = -0			
0	6	147	153
0	7	58	64
0	8	42	44
0	9	72	75
0	10	39	39
0	11	74	77
0	13	53	54
-1	3	145	148
-1	4	29	28
-1	5	141	145
-1	6	51	49
-1	7	123	127
-1	9	92	93
-1	10	47	47
-1	11	60	60
-1	11	63	65
-1	12	32	35
-1	13	36	36
-1	13	41	36
-2	0	89	85
-2	1	94	99
-2	1	53	58
-2	3	108	108
-2	3	45	49
-2	4	85	90
-2	5	46	46
-2	6	109	112
-2	7	59	63
-2	8	96	98
-2	9	23	23
-2	10	98	99
-2	12	59	62
-3	0	150	150
-3	1	88	88
-3	2	120	126
-3	2	156	159
-3	3	109	113
-3	4	37	38
-3	4	91	97
-3	5	111	111
-3	6	26	29
-3	6	81	83
-3	7	148	149
-3	8	82	84
-3	9	54	54
-3	10	43	42
-3	11	33	36
-4	0	163	163
-4	1	88	89
-4	1	73	70
-4	2	141	146
-4	2	117	121
-4	3	27	24
-4	3	49	48
-4	4	163	167
-4	4	80	79
-4	5	54	53
-4	5	72	75
-4	6	93	95
-4	6	39	37
-4	7	35	34
-4	7	77	73
-4	8	70	70
-4	9	52	55
-4	10	91	89
-4	11	73	71
-4	11	40	34
-4	12	34	35
-5	0	47	47
-5	1	85	82
-5	1	120	120
-5	2	49	49
-5	2	38	39
-5	3	143	144
-5	3	96	97
-5	4	154	159
-5	4	59	55
-5	5	77	80
1	-3	44	47
-1	4	45	49
-1	-4	128	129
-1	5	78	77
1	-5	62	64
-1	-6	35	41
-1	6	64	59
1	-6	123	122
-1	-7	51	99
-1	7	47	49
1	-7	79	82
-1	-8	78	86
-1	8	73	75
1	-8	59	58
-1	-9	41	47
1	-9	92	95
-1	-10	66	67
-1	10	57	57
1	-11	31	38
1	-11	50	53
1	-12	50	45
-1	-12	43	45
-1	12	51	46
1	-13	39	36
1	-13	50	55
2	0	69	70
-2	0	125	125
2	1	44	42
-2	-1	110	110
2	1	172	172
2	-1	151	153
2	2	44	42
2	2	65	66
2	3	53	93
-2	3	44	42
2	-3	172	169
2	4	109	109
-2	4	80	82
-2	-5	134	135
-2	-6	54	54
-2	6	32	50
-2	-7	127	131
2	-7	130	134
-2	-8	25	28
-2	8	68	67
-2	-9	85	90
-2	9	41	41
-2	-9	109	107
-2	-10	22	25
-2	10	60	65
-2	-10	30	30
-2	-11	85	82
-2	11	31	27
-2	-11	49	49
-2	-12	27	32
-2	-12	44	42
-2	-13	59	63
3	0	53	54
-3	0	141	140
-3	1	109	110
-3	-1	40	39
-3	1	80	80
3	-1	165	166
3	2	68	70
-3	-2	64	66
3	2	128	130
3	-3	55	54
3	3	135	133
-3	-3	61	60
-3	3	83	84
-3	-3	94	95
-3	-4	140	141
-3	4	52	51
3	-4	78	78
3	5	155	158
-3	5	45	45
-3	5	56	60
3	-5	41	46
-3	-6	91	93
-3	6	74	76
3	-6	86	89
3	7	110	111
6	4	54	52
-6	-4	42	41
-6	4	41	42
6	5	64	68
-6	-5	67	65
-6	5	38	37
6	-5	73	69
6	6	73	74
-6	-6	58	59
6	-6	39	37
6	7	38	37
-6	-7	65	66
-6	7	30	31
6	8	86	89
-6	-8	47	47
6	9	40	35
-6	-9	82	81
6	-9	49	46
6	10	103	106
-6	-10	37	33
-6	-11	76	79
6	12	71	66
-6	-13	46	48
-7	0	65	65
-7	0	35	39
7	1	60	60
-7	-1	55	55
7	1	66	65
7	-1	49	50
7	2	53	55
-7	-2	50	47
7	-2	52	53
7	3	104	100
-7	3	41	46
7	-3	51	48
-7	-4	69	69
7	-4	54	56
7	5	104	102
-7	5	52	52
7	6	29	32
-7	-6	41	38
7	-6	48	50
7	7	100	102
-7	-8	66	66
7	9	75	75
7	10	31	31
-7	-10	65	62
-7	-11	55	60
-7	-11	52	49
-7	12	39	38
-7	-12	32	27
-7	13	35	36
-7	-13	45	40
8	0	79	77
-8	-1	62	57
-8	1	52	53
8	2	100	98
8	-2	62	63
8	3	50	47
-8	-3	66	70
-8	3	45	52
8	4	82	80
-8	-4	30	33
8	-5	51	54
-8	5	41	37
8	6	91	92
8	7	40	35
8	8	68	75
-8	-8	52	54
-8	9	54	57
-8	-9	37	38
-8	10	32	31
-8	-10	37	38
-8	11	47	46
-8	-12	46	44
8	13	41	40
9	1	48	48
-9	-1	46	44
9	-1	35	32
9	2	51	48
-9	-3	45	45
9	-3	45	48
-3	0	22	18
3	1	130	130
-3	-1	60	60
-3	1	108	104
3	-1	110	112
3	2	90	88
-3	-2	67	67
-3	2	45	43
3	-2	54	56
3	3	62	64
-3	-3	46	43
-3	3	97	96
3	-3	98	99
3	4	33	34
-3	-4	69	69
3	5	119	119
-3	-5	61	60
-3	5	87	86
3	-5	69	73
3	6	63	65
-3	-6	115	115
-3	7	31	35
3	-7	60	58
-3	-7	44	44
3	8	46	46
-3	-8	54	60
-3	9	67	68
3	-9	56	58
3	10	48	48
-3	-10	62	64
3	-10	53	54
-3	11	33	31
-3	-12	48	47
-4	0	44	49
4	1	80	84
-4	-1	81	91
-4	1	94	91
4	-1	93	92
-4	-2	63	67
-4	2	23	26
4	-2	45	44
4	3	103	108
-4	-3	94	92
-4	3	109	109
4	-3	49	51
-4	-4	47	45
-4	4	56	58
4	-4	62	61
4	5	95	93
4	-5	88	87
-4	5	46	42
-4	6	43	41
4	-6	42	41
4	7	50	51
-4	-7	33	40
-4	7	27	28
4	8	23	21
4	-8	52	53
4	9	76	78
-4	-9	24	26
-4	-10	35	37
-4	10	41	48
4	-10	61	55
4	-11	55	57
-4	-11	45	44
-4	-12	58	62
-5	0	61	63
-5	0	41	42
-5	2	58	60
-5	-2	51	56
5	-2	69	71
-5	-2	66	69
5	3	44	47
-5	-3	64	70
5	-3	43	42
5	4	39	38
5	4	50	49
-5	-4	95	97
5	4	67	62
-5	-4	51	51
5	-5	31	34
-5	-5	37	35
9	10	36	31
9	11	40	39
-10	1	32	32
10	3	36	31
-10	-6	40	38
10	8	33	40
-10	-8	56	55
-10	-10	35	36
K = 3			
0	0	27	28
0	1	115	112
0	2	126	122
-0	-2	69	68
0	4	131	122
0	5	23	22
-0	-5	52	53
0	6	68	68
0	7	70	66
-0	-7	63	65
0	8	88	89
-0	-9	40	45
0	10	52	52
-0	-11	30	28
0	12	44	40
-0	-13	29	27
1	0	51	48
-1	0	257	239
1	1	71	71
-1	-1	76	69
1	-1	122	125
1	2	56	54
-1	-2	55	54
-1	2	207	194
-1	-3	59	53
-1	3	60	54
1	4	33	30
-1	-4	44	46
-1	4	80	76
-1	-5	95	94
-1	5	28	30
1	6	33	35
1	-6	39	37
-1	6	78	80
1	-6	64	65
1	7	98	97
1	-7	75	78
1	8	30	36
-1	-8	54	49
1	8	26	26
1	-8	61	60
1	9	47	51
-1	-9	48	48
1	9	43	46
1	10	74	72
1	-10	46	49
1	11	53	56
-1	11	24	26
-1	-13	45	46
-1	13	35	32
-2	0	39	41
-2	0	107	112
-2	1	168	160
2	1	38	35
-2	-2	59	60
2	2	62	63
-2	-2	30	38
-2	-3	75	74
2	3	66	74
-2	-4	57	54
2	4	92	95
-2	-4	79	77
2	5	137	130
-2	-5	59	65
-2	5	24	28
2	-6	50	51
-2	6	97	95
2	-6	47	42
2	7	54	55
-2	7	68	70
-2	7	85	81
5	-8	32	25
5	9	58	59
-5	9	53	51
-5	-10	49	53
5	11	70	68
-5	-11	35	36
-5	11	45	41
-5	12	43	41
-5	-13	30	28
-5	13	37	39
-5	-13	45	45
6	0	46	47
-6	0	37	38
6	1	25	21
-6	-1	68	70
-6	1	74	72
6	2	63	67
-6	-2	59	61
-6	2	37	35
6	-3	53	48
-6	3	86	88
-6	3	56	58
6	4	63	62
-6	-4	76	76
6	-4	43	41
-6	-5	43	44
-6	5	74	76
-6	-6	49	52
-6	6	36	37
6	-6	44	41
6	7	35	37
-6	-7	35	36
-6	7	55	55
6	8	29	27
-6	-8	45	46
6	9	46	45
-6	-9	45	50
-6	9	29	32
-6	-10	46	46
6	-11	43	35
-6	-12	31	33
6	13	49	50
7	0	29	33
-7	0	60	64
-7	-1	58	59
-7	1	37	39
-7	2	47	46
7	-2	34	34
7	3	46	48
-7	-3	73	76
7	3	43	42
7	4	41	42
-7	4	49	50
-7	-5	48	52
-7	5	36	33
-7	6	37	37
-7	6	56	58
7	-7	63	61
-7	8	30	31
-7	-8	23	24
-7	8	34	38
-7	-9	64	65
7	10	42	40
-7	-11	26	28
-7	-13	30	28
-8	0	72	70
-8	2	55	60
-8	-3	36	32
-8	-4	54	50
-8	4	49	51
-8	-5	36	37
8	6	28	28
-8	-6	54	52
-8	6	41	41
8	-7	45	50
8	-7	36	38
-8	-8	47	45
8	9	50	49
-8	-9	41	41
-8	-11	32	31
-8	-13	36	40
-9	0	43	44
2	-3	64	63
-2	4	34	34
2	-4	53	56
2	-5	101	105
-2	-5	102	99
-2	5	110	111
2	-5	48	45
-2	-6	50	53
2	6	26	22
2	-6	46	44
2	7	106	107
-2	-7	54	54
-2	7	78	78
2	-7	39	41
-2	-8	55	54
-2	-8	35	38
-2	8	52	52
2	-8	51	53
2	9	55	59
-2	-9	41	43
-2	9	47	44
2	10	54	51
-2	10	88	82
2	11	62	59
2	12	45	45
-2	12	63	59
3	0	103	103
-3	0	85	80
-3	-1	62	61
-3	1	68	71
3	-1	34	35
3	2	67	72
-3	-2	67	71
3	2	103	101
3	-2	82	87
-3	-3	58	85
-3	3	31	33
3	4	25	67
-3	-4	65	64
-3	4	133	132
3	-4	53	51
3	5	103	98
-3	-5	128	127
3	6	51	54
-3	-6	32	32
-3	6	50	94
3	-6	33	37
3	7	70	73
-3	-7	108	103
-3	-8	36	33
-3	8	99	102
3	9	56	57
-3	-9	73	70
-3	9	38	41
3	10	30	27
-3	10	83	82
3	11	81	81
-3	-11	64	70
-3	11	40	42
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-5	7	35	39
-5	-8	52	49
-5	-10	50	43
-5	11	55	46
-6	-1	45	42
-6	1	60	64
-6	2	34	34
6	3	33	26
-6	-3	52	56
-6	3	70	69
-6	-4	30	37
6	5	48	43
-6	5	34	31
6	6	33	31
-6	7	39	34
-6	-7	42	44
-6	7	40	41
-6	8	50	49
6	-9	46	35
-6	-10	35	37
-7	0	56	58
-7	-2	52	51
-7	2	63	65
-7	-3	55	55
-7	3	32	33
-7	-4	37	42
-7	4	36	32
-7	-5	30	26
-7	-6	40	49
-7	-7	32	31
-7	-8	44	42
-7	8	30	33
-7	-9	43	39
-8	-2	69	69
-8	2	34	37
-8	3	39	37
-8	-4	53	53
-8	4	41	42
-8	-6	46	48
-8	7	41	38
-8	-8	56	54
-9	1	47	45
-9	2	38	32
-9	3	36	35
-9	-4	38	34
-9	5	44	50
-9	-6	49	45
-9	-8	37	38
-10	-3	38	39
K = 9			
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-0	-2	71	73
-0	-3	36	38
-0	-4	42	43
0	5	37	36
0	6	51	51
-0	-6	54	57
0	7	72	72
0	8	46	49
0	9	75	80
0	10	40	41
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1	1	40	38
-1	-1	33	32
-1	1	69	71
1	-1	30	31
1	2	59	66
1	3	54	37
-1	-3	57	54
-1	3	72	71
-1	4	49	50
-1	-4	52	53
-1	-5	36	36
1	5	56	57
1	-5	32	31
1	6	65	67
-1	-6	46	46
-1	7	83	82
1	8	61	61
1	8	71	66
1	9	68	66
1	10	42	37
-1	10	60	66
-1	11	51	51
-2	0	40	43
-2	1	73	73
2	-1	56	52
-2	2	50	45
2	-2	32	27
2	3	53	50
-2	-3	34	38
-2	3	54	53
-2	4	72	75
2	5	40	36
-2	-5	58	54
-2	5	27	26
-2	6	41	47
-2	6	68	71
-2	7	40	40
-2	-7	35	35
-2	8	48	47
-2	8	83	75
2	9	29	25
-2	10	54	55
-2	10	70	70
-3	0	58	95
-3	-2	50	51
-3	2	102	99
-3	3	36	34
-3	-4	70	71
-3	4	73	75
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-3	-5	39	35
-3	6	66	67
-3	7	57	61
-3	7	46	45
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-3	11	50	50
-3	11	50	48
-4	0	45	42
-4	-1	51	49
-4	1	51	52
4	2	37	37
-4	-2	64	64
-4	2	71	70
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-4	3	48	53
4	4	45	47
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-4	-6	63	57
-4	7	79	78
4	8	36	29
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4	9	31	33
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4	10	36	36
4	11	41	44
-4	11	54	57
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-5	-4	54	46
-5	-5	62	61
-5	5	71	76
5	-6	47	44
-5	-6	62	64
-5	6	57	56
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5	7	42	41
-5	8	35	39
-5	-8	44	41
-5	8	52	50
-5	-9	40	37
-5	10	51	51
-6	0	70	66
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-6	3	47	45
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6	7	36	32
-6	-7	53	53
-6	8	50	62
-6	-9	41	48
-7	0	55	94
-7	1	36	37
-7	-2	84	81
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-7	4	78	79
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-7	-6	42	42
-7	6	47	46
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-9	-9	62	59
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-10	-4	50	52
-11	0	45	48
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0	-2	39	41
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-0	-3	41	38
0	-5	88	85
-0	-5	40	34
0	7	95	96
0	9	61	65
0	10	53	53
0	11	52	54
1	0	75	72
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-1	1	48	50
-1	-1	92	89
1	2	82	82
1	3	58	54
-1	-3	54	54
-1	3	65	68
1	4	67	65
1	5	53	56
-1	-5	62	61
1	5	45	49
1	6	76	75
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-1	7	39	35
-1	8	32	35
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-2	-1	41	41
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-2	-3	46	44
2	-3	42	40
2	4	59	60
-2	-4	44	43
-2	4	77	81
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-2	-6	38	34
-2	6	78	79
-2	-7	58	55
-2	7	31	30
2	8	68	71
-2	8	76	81
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-2	10	45	50
-2	11	56	51
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-3	-1	41	45
-3	-2	58	96
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-3	-8	44	46
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-4	-7	69	63
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-4	8	53	49
4	9	37	43
-4	-9	44	42
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5	0	38	36
-5	0	61	56
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-6	-6	44	43
-6	6	78	71
-6	7	64	67
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-6	-9	41	39
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-7	-3	41	41
-7	3	74	79
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-7	7	53	54
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-8	-7	50	50
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-9	4	43	48
-9	-5	52	50
-9	-7	61	62
-10	0	45	48
-10	-4	58	62
K = 11			
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0	3	66	70
-0	-3	59	60
0	4	33	35
0	5	67	67
0	7	38	38
0	8	61	62
1	0	56	59
-1	1	37	34
1	-1	47	48
-1	-2	37	36
-1	2	69	75
1	3	66	64
-1	-3	44	47
-1	4	59	63
1	5	75	76
-1	-5	46	52
1	6	57	60
1	7	74	74
-1	8	56	64
-1	9	62	63
-1	9	34	36
-2	0	57	56
-2	0	56	59
2	2	63	61
-2	-2	53	54
-2	3	68	70
2	3	56	56
-2	4	54	52
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-2	-6	57	59
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-2	7	61	56
2	8	58	60
-2	9	41	39
-2	9	56	59
-2	9	64	66
-3	0	36	35
-3	-1	58	62
-3	1	83	90
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-3	3	59	54
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-3	-4	42	35
-3	-5	46	39
3	5	72	74
3	6	61	59
-3	-6	48	46
-3	7	55	56
-3	0	59	58
-3	9	51	55
-4	0	38	40
-4	-1	55	56
-4	1	62	64
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-6	-4	59	60
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-6	-6	66	60
-6	7	42	40
-7	-1	55	57
-7	1	46	53
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-7	3	59	61
-7	4	31	26
-7	-5	41	43
-7	5	41	46
-7	6	40	43
-7	-7	50	46
-8	0	48	49
-8	-1	44	45
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-8	2	49	49
-8	-3	52	52
-8	4	46	45
-9	0	53	48
-9	-2	50	59
-9	-4	45	47
K = 12			
0	0	47	49
0	2	55	58
0	4	42	44
0	6	42	43
0	8	47	47
-1	0	56	54
-1	1	51	51
-1	2	55	50
1	6	43	40
1	7	47	45
1	8	39	45
-2	-1	31	33
-2	1	48	48
-2	3	52	53
-2	5	42	44
-2	7	39	42
-2	9	38	40
-3	0	42	45
-3	3	46	47
-3	4	55	57
-3	6	50	48
-3	8	45	43
-4	0	53	54
-4	2	61	57
-4	4	55	58
-4	8	32	35
-5	0	32	32
-5	2	38	43
-5	3	32	28
-6	-1	42	43
-6	3	41	43
-6	5	34	40
-7	0	33	31
-7	2	41	44
-7	4	44	44
-8	0	36	39
K = 13			
-4	0	35	35

TABLE 2

POSITIONAL AND THERMAL PARAMETERS OF NONGROUP ATOMS[a–c]

Atom	x/a	y/b	z/c	β_{11}	β_{12}	β_{13}	β_{22}	β_{23}	β_{33}
Re	−1409(1)	1165(1)	2669(0)	74(1)	55(1)	−47(1)	41(0)	−32(0)	36(0)
S(1)	1231(4)	2129(3)	2104(3)	86(4)	53(6)	−74(6)	72(3)	−50(5)	80(3)
S(2)	−459(4)	1052(3)	4058(3)	189(6)	149(8)	−141(7)	91(4)	−73(5)	59(3)
P(1)	−1182(3)	−705(3)	2606(2)	91(4)	74(5)	−48(5)	46(3)	−33(4)	35(2)
P(2)	−1598(3)	3024(3)	2788(2)	70(4)	42(5)	−38(5)	44(3)	−32(4)	37(2)
O(1)	−4585(10)	64(8)	3788(8)	69(13)	43(17)	13(16)	79(9)	8(13)	74(8)
O(2)	−1830(11)	1342(8)	704(8)	177(17)	104(21)	−77(17)	97(10)	−43(13)	44(7)
C(1)	−3409(16)	455(10)	3346(10)	135(22)	60(23)	−91(23)	25(10)	−11(15)	46(9)
C(2)	−1685(12)	1308(10)	1447(11)	76(17)	54(20)	−39(19)	43(10)	−21(15)	53(10)
C(3)	1162(16)	1745(14)	3227(13)	129(22)	105(30)	−109(28)	91(15)	−96(24)	10(15)

[a] All values × 10^4. [b] The β_{ij} are the coefficients of the form: $h^2\cdot\beta_{11}+k^2\cdot\beta_{22}+l^2\cdot\beta_{33}+h\cdot k\cdot\beta_{12}+h\cdot l\cdot\beta_{13}+k\cdot l\cdot\beta_{23}$. [c] The numbers in parentheses here and in the succeeding tables are the esd's on last significant digits.

TABLE 3

RIGID-GROUP PARAMETERS AND MEAN ISOTROPIC TEMPERATURE FACTORS OF PHENYL RINGS[a,b]

Group	x/a	y/b	z/c	α (°)	β (°)	γ (°)	B (Å^2)
P(1)R(1)	−2810(6)	−2106(5)	1137(4)	141.7(3)	−25.6(3)	158.2(3)	4.0(1)
P(1)R(2)	2339(6)	−419(5)	1971(5)	69.9(11)	74.9(2)	164.7(11)	3.9(1)
P(1)R(3)	−2746(6)	−2966(5)	4644(4)	−76.1(4)	33.5(2)	−63.4(4)	3.7(1)
P(2)R(1)	−4242(6)	3709(5)	2125(4)	16.7(3)	12.9(3)	−97.4(2)	3.4(1)
P(2)R(2)	−2286(6)	3262(5)	5147(4)	−105.7(3)	6.6(2)	15.2(3)	3.8(1)
P(2)R(3)	1139(6)	5509(5)	1306(4)	111.8(5)	47.4(3)	−88.2(4)	4.1(1)

[a] $(x/a, y/b, z/c)\times 10^{-4}$ is the displacement vector of the center of gravity of a phenyl ring from the cell origin. [b] α, β and γ are the arguments of anticlockwise rotations around three orthogonal axes X, Y and Z (X is in the plane of a and b, Y coincides with b); the phenyl ring in the initial position lies on XY plane with atoms C(1) and C(4) [the latter in *para* to C(1)] on the Y axis.

RESULTS AND DISCUSSION

The final list of computed and observed structure factor moduli, in electrons, is given in Table 1. Table 2 gives the positional and thermal co-ordinates of all non-group atoms; Tables 3 and 4 list the group parameters and the individual co-ordinates for the atoms treated in rigid groups; bond distances and angles are reported in Table 5, whereas Table 6 gives the r.m.s. displacements for all the atoms which have been treated anisotropically.

The structure consists of a packing of discrete monomeric molecules. A survey of all possible inter-molecular contacts does not reveal any unusual features.

The molecule, as shown in Fig. 1, displays a distorted octahedral co-ordination around the metal atom. Two *cis* positions are occupied by the sulphur atoms of the CS_2 group which chelates on the metal atom thereby closing a four membered ring; the two CO groups occupy the pair of positions *trans* to the sulphur atoms; the phosphine groups, *trans* one to the other, complete the octahedron. This scheme of

TABLE 4

POSITIONAL PARAMETERS OF PHENYLIC CARBON ATOMS[a,b]

Atom	*x/a*	*y/b*	*z/c*	Atom	*x/a*	*y/b*	*z/c*
C(111)	−1995(9)	−1444(10)	1789(7)	C(211)	−3042(9)	3359(8)	2452(7)
C(112)	−3375(9)	−1501(7)	1885(6)	C(212)	−3953(9)	2588(6)	2116(7)
C(113)	−4076(7)	−2070(8)	1323(6)	C(213)	−4988(7)	2890(6)	1835(6)
C(114)	−3397(8)	−2584(8)	666(6)	C(214)	−5109(7)	3962(6)	1889(6)
C(115)	−2019(8)	−2526(7)	570(6)	C(215)	−4197(8)	4733(5)	2225(6)
C(116)	−1317(7)	−1957(9)	1132(7)	C(216)	−3164(8)	4430(7)	2506(7)
C(121)	664(11)	−630(37)	2256(7)	C(221)	−1930(9)	3199(9)	4032(5)
C(122)	1537(11)	−220(25)	1294(6)	C(222)	−836(7)	3518(8)	4411(5)
C(123)	2979(8)	−39(10)	1048(5)	C(223)	−1145(7)	3573(7)	5372(6)
C(124)	3547(9)	−268(27)	1765(6)	C(224)	−2544(8)	3306(7)	5952(4)
C(125)	2674(9)	−677(16)	2728(5)	C(225)	−3635(6)	2987(7)	5573(5)
C(126)	1232(8)	−858(19)	2974(5)	C(226)	−3328(8)	2933(8)	4612(6)
C(131)	−2033(12)	−1888(6)	3700(5)	C(231)	−99(13)	4347(8)	2040(6)
C(132)	−1940(8)	−2964(7)	3627(4)	C(232)	533(13)	4352(6)	1084(7)
C(133)	−2552(10)	−3892(6)	4440(6)	C(233)	1597(8)	5352(7)	451(5)
C(134)	−3260(10)	−3744(6)	5326(5)	C(234)	2031(10)	6347(7)	776(5)
C(135)	−3354(8)	−2668(7)	5400(5)	C(235)	1401(11)	6342(6)	1731(6)
C(136)	−2739(12)	−1739(6)	4587(6)	C(236)	336(9)	5343(8)	2363(5)

[a] All values × 10^4. [b] Atoms from C(111) to C(116) belong to the phenyl P(1)R(1).

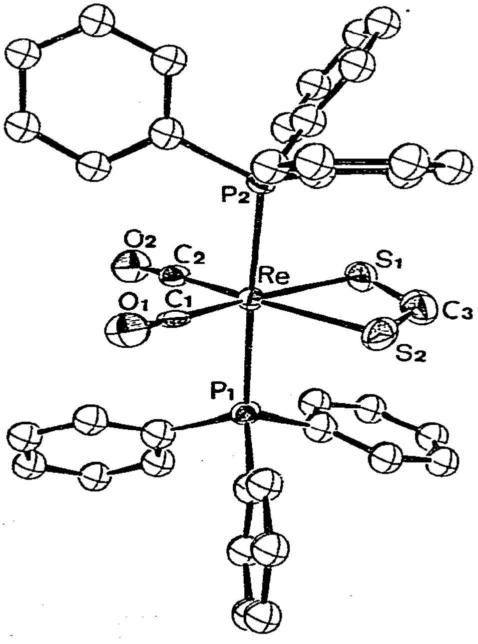


Fig. 1. Overall view by ORTEP of the molecule $Re(HCS_2)(CO)_2[P(C_6H_5)_3]_2$. The ellipsoids have been drawn at 40% probability.

coordination allows the minimum interaction between two bulky PR_3 ligands and is probably adopted because of this.

TABLE 5

DISTANCES (Å) AND ANGLES (°) WITHIN THE MOLECULE Re(CO)$_2$(HCS$_2$)[P(C$_6$H$_5$)$_3$]$_2$

Bonds involving the rhenium atom			
Re–S(1)	2.500(3)	S(1)–Re–C(1)	168.7(5)
Re–S(2)	2.532(5)	S(1)–Re–C(2)	99.1(3)
Re–P(1)	2.426(4)	S(2)–Re–P(1)	85.4(1)
Re–P(2)	2.412(4)	S(2)–Re–P(2)	92.2(1)
Re–C(1)	1.91(1)	S(2)–Re–C(1)	100.8(5)
Re–C(2)	1.91(2)	S(2)–Re–C(2)	99.6(2)
S(1)–Re–S(2)	68.4(1)	P(1)–Re–C(1)	91.6(4)
P(1)–Re–P(2)	177.6(1)	P(1)–Re–C(2)	90.4(4)
C(1)–Re–C(2)	91.9(6)	P(2)–Re–C(1)	88.8(4)
SS(1)–Re–P(1)	90.8(1)	P(2)–Re–C(2)	92.0(4)
S(1)–Re–P(2)	88.3(1)		
Bonds involving the dithioformato ligand			
S(1)–C(3)	1.64(2)	Re–S(1)–C(3)	88.3(5)
S(2)–C(3)	1.68(1)	Re–S(2)–C(3)	86.5(7)
S(1)–C(3)–S(2)	116.7(1)		
Bonds involving the carbonyl ligands			
C(1)–O(1)	1.14(2)	Re–C(1)–O(1)	176(1)
C(2)–O(2)	1.15(2)	Re–C(2)–O(2)	176(1)
Bonds involving the phosphine ligands			
P(1)–C(111)	1.86(1)	P(1)–C(111)–C(114)	175.9(5)
P(1)–C(121)	1.83(2)	P(1)–C(121)–C(124)	173.0(9)
P(1)–C(131)	1.83(1)	P(1)–C(131)–C(134)	177.5(6)
P(2)–C(211)	1.86(1)	P(2)–C(211)–C(214)	177.2(4)
P(2)–C(221)	1.85(1)	P(2)–C(221)–C(224)	176.2(5)
P(2)–C(231)	1.84(1)	P(2)–C(231)–C(234)	174.4(7)
Re–P(1)–C(111)	114.8(4)	C(111)–P(1)–C(121)	107(1)
Re–P(1)–C(121)	112.8(9)	C(111)–P(1)–C(131)	98.8(4)
Re–P(1)–C(131)	119.1(3)	C(121)–P(1)–C(131)	102(1)
Re–P(2)–C(211)	117.2(3)	C(211)–P(2)–C(221)	103.4(5)
Re–P(2)–C(221)	112.0(4)	C(211)–P(2)–C(231)	98.8(5)
Re–P(2)–C(231)	118.7(4)	C(221)–P(2)–C(231)	104.7(4)
Most relevant non-bonding distances			
Re–C(3)	2.95(2)	S(1)–C(2)	3.38(2)
Re–O(1)	3.05(1)	S(2)–C(1)	3.45(2)
Re–O(2)	3.06(1)	P(1)–C(1)	3.13(2)
S(1)–S(2)	2.830(5)	P(1)–C(2)	3.10(2)
S(1)–P(1)	3.508(5)	P(2)–C(1)	3.05(1)
S(1)–P(2)	3.423(6)	P(2)–C(2)	3.13(1)
S(2)–P(1)	3.365(6)	C(1)–C(2)	2.75(2)
S(2)–P(2)	3.563(6)		

Apart from the phenyl rings, the symmetry of the molecule is approximately C_{2v}, with the twofold axis bisecting the angles S(1)–Re–S(2) and C(1)–Re–C(2) and the two planes passing through Re, S(1), S(2), C(1), C(2), C(3) and, respectively, Re, P(1), P(2), C(3). The angle between the "best planes"[12] defined by the two sets of atoms is 86.4(1)°.

Although in the final Fourier difference no signals indicating an hydrogen

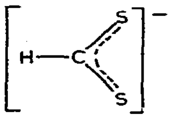
TABLE 6

ROOT-MEAN-SQUARE DISPLACEMENTS (Å) OF PRINCIPAL AXES OF THERMAL ELLIPSOIDS FOR NON-GROUP ATOMS

Atom	Axis 1	Axis 2	Axis 3	Mean esd.
Re	0.148	0.166	0.195	0.001
S(1)	0.187	0.220	0.280	0.006
S(2)	0.181	0.215	0.307	0.007
P(1)	0.149	0.177	0.209	0.007
P(2)	0.159	0.176	0.195	0.007
O(1)	0.16	0.23	0.31	0.02
O(2)	0.20	0.25	0.28	0.02
C(1)	0.11	0.19	0.26	0.03
C(2)	0.16	0.19	0.23	0.03
C(3)	0.21	0.22	0.32	0.03

atom associated with the CS_2 group were observed there are a number of reasons to believe that the hydrido ligand of the parent $ReH(CO)_2[P(C_6H_5)_3]_2$ has been transferred to the carbon atom of the entering CS_2 molecule, which thus becomes a dithioformato ligand.

The following considerations favour such a view. Firstly, it has been shown that CS_2 in itself bonds to metal atoms via one S atom and the C atom, the bonded group being merely the molecule in its first excited state[13]. The substantial equivalence of the S–C and Re–S bonds in the present complex (however, see below for a possible disorder) indicates that the electron density is the same on both sulphur atoms and supports an electronic distribution similar to that of carboxylate anions:



The four-membered ring is comparable with similar rings in complexes of anions of a number of dithio acids and dithiocarbamic acids. A survey of recent structural reports on such compounds* shows that very often the chelate ring possesses equivalent C–S bonds; in dithiocarbamates the distances vary from 1.66Å to 1.80 Å, most of them falling around 1.70 Å; in chelating anions of dithioacids this spread is from 1.58 Å to 1.72 Å. In both classes of compounds the S–C–S angle is in a range of 110°–120°. So, from the point of view of the bonding parameters, the chelate group observed in this structure, with distances C–S of 1.64(2) Å and 1.68(1) Å and an angle of 116.7(1)°, is a typical dithioanion.

These arguments are consistent with the observed diamagnetism of the complex and with the fact that no NMR signals assignable to a Re–H interaction could be detected[2]. On the other hand, a coordinated hydrido ion would have significantly distorted the observed coordination pattern.

In the light of this result, the isoelectronic Rh^{III} and the Ir^{I} compounds referred

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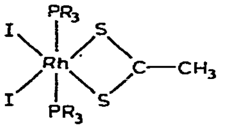
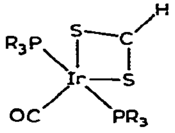
* For recent structural determinations on metal dithiocarbamates and on metal dithiocarboxylates see refs. 14 and 15, respectively.

upon in the introduction can be considered as the hexacoordinated (I) and the pentacoordinated (II) complexes shown below:



(I)



(II)

Structural reports on Re complexes are relatively scarce so that comparison of the data on the Re–S, Re–P and Re–CO bonds with those previous obtained is informative. No data on Re–S bond lengths were available until very recently, but comparison could be made with the structure of $Mo(NO)[S_2CN(C_4H_9)_2]_3$ (ref. 16). In this compound the six Mo–S interactions (2.53 Å to 2.57 Å) are comparable with those found here [2.500(3) Å to 2.532(5) Å]. While we were writing this article however, results have been published of a structural investigation into two Re^V dithiocarbamates: $Re_2O_3[S_2CN(C_2H_5)_2]_4$ and $ReN[S_2CN(C_2H_5)_2]_2$[17]; the ranges reported for the Re–S distances are 2.40–2.47 Å and 2.38–2.39 Å, respectively.

The metal phosphorus distances in this structure [2.426(4) Å and 2.412(4) Å] are to be compared with the values of: 2.34 Å in $ReH_3[P_2(C_6H_5)_4(C_2H_4)]_2$[18], 2.36–2.39 Å in $ReH_3[P(C_6H_5)_3]_2[P_2(C_6H_5)_4(C_2H_4)]$[19], 2.45–2.48 Å in $ReOCl_3[P(C_2H_5)_2(C_6H_5)]_2$[20], 2.45 Å in $ReNCl_2[P(C_6H_5)_3]_2$[21], and, lastly, 2.44–2.49 Å in $ReNCl_2[P(C_2H_5)_2(C_6H_5)]_3$[22].

As for the Re–C–O interactions, the Re–C distances of 1.91 (1) and 1.91 (2) Å and the CO distances of 1.14(2) and 1.15(2) Å are to be compared with the following (mean) values: 1.89 Å and 1.16 Å in $[(B_9C_2H_{11})Re(CO)_3]^-$ [23], 1.91 Å and 1.19 Å in $[Re_4(CO)_{16}]^{2-}$ [24], 1.95 Å and 1.15 Å in $Re_2MnH(CO)_{14}$[25], and 2.00 Å and 1.12 Å in $Tc_2(CO)_{10}$[26].

In the complex we examined there are, however, indications of disorder concerning to Re–C–O interactions. As can be seen in Fig. 2, the directions of the maximum *apparent* displacements of both carbon atoms, almost coincident with the Re–C and the C–O bonds, is contrary to what would be expected on the basis of stretching and bending energies. The observed situation can be interpreted as an averaging of different Re–C and C–O bonds. Apparently this disorder does not affect the oxygen atoms, the thermal ellipsoids for which show the expected orientation. This happens, probably, because in a metal–carbonyl interaction an increase of the M–C distance (bond order decreasing) causes a shortening of the C–O distance (bond order increasing) and *vice versa*, so that the positional parameters of the oxygen atom probably remain relatively unaffected by such a disorder in the position of the carbon atom.

A peculiar feature is also present in the thermal motion of the HCS_2^- group. Here, the orientations of the three thermal ellipsoids suggest either that the group is rocking as whole around the metal atom or that two actually different C–S bonds are averaged by a disorder. It is not possible, from the present data, to decide between the two models; the effect is probably connected with the disorder in the CO groups which are *trans* to the sulphur atoms.

We intend to continue the investigation into these kinds of complex with a dual purpose, to collect more data on the structures of complexes of addition of CS_2

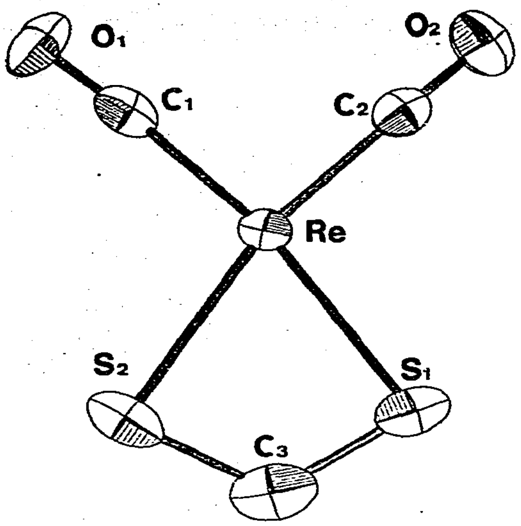


Fig. 2. An ORTEP drawing of the $Re(HCS_2)(CO)_2$ moiety. Thermal ellipsoids at 40% probability.

and of related species and also to elucidate if possible the nature of the disorder observed in the structure described above.

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