Table 1. Crystal data and structure refinement for $Cs_2Pt(CN)_4*0.75H_2O$.

| | |
|---|---|
| Empirical formula | $Cs_2Pt(CN)_4O_{0.75}$ |
| Formula weight | 576.99 |
| Temperature | 100(2) K |
| Wavelength | 0.7000 Å |
| Crystal system | Monoclinic |
| Space group | $P2_1/c$ |
| Unit cell dimensions | a = 9.40820(10) Å |
| | b = 20.8216(4) Å β= 119.410(2)°. |
| | c = 17.9431(3) Å |
| Volume | 3061.96(8) $Å^3$ |
| Z | 12 |
| Density (calculated) | 3.755 $g/cm^3$ |
| Absorption coefficient | 20.735 $mm^{-1}$ |
| F(000) | 2952 |
| Crystal size | 0.16 x 0.05 x 0.01 $mm^3$ |
| Theta range for data collection | 1.63 to 30.51°. |
| Index ranges | $-13 \le h \le 13$, $-29 \le k \le 29$, $-24 \le l \le 25$ |
| Reflections collected | 56894 |
| Independent reflections | 9340 [R(int) = 0.0406] |
| Completeness to theta = 30.51° | 99.8 % |
| Absorption correction | SADABS |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 9348 / 0 / 352 |
| Goodness-of-fit on $F^2$ | 1.034 |
| Final R indices [I>2sigma(I)] | R1 = 0.0290, wR2 = 0.0728 |
| R indices (all data) | R1 = 0.0326, wR2 = 0.0745 |
| Largest diff. peak and hole | 2.822 and -4.528 $e.Å^{-3}$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for $Cs_2Pt(CN)_4$*$0.75H_2O$. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Pt(1) | 5320(1) | 2252(1) | 3719(1) | 24(1) |
| C(11) | 3632(7) | 1921(3) | 3998(4) | 31(1) |
| C(12) | 7059(7) | 1979(3) | 4887(4) | 34(1) |
| C(13) | 6946(7) | 2571(3) | 3394(4) | 34(1) |
| C(14) | 3583(7) | 2518(3) | 2547(4) | 30(1) |
| N(11) | 2686(7) | 1730(3) | 4176(4) | 42(1) |
| N(12) | 8011(8) | 1822(3) | 5569(4) | 49(2) |
| N(13) | 7830(7) | 2782(4) | 3176(4) | 49(2) |
| N(14) | 2620(6) | 2696(3) | 1870(3) | 41(1) |
| Pt(2) | 5139(1) | 3643(1) | 4345(1) | 17(1) |
| C(21) | 7568(6) | 3713(3) | 4984(3) | 23(1) |
| C(22) | 5246(6) | 3244(2) | 5391(3) | 20(1) |
| C(23) | 2690(6) | 3570(2) | 3698(3) | 20(1) |
| C(24) | 5057(6) | 4057(2) | 3316(3) | 20(1) |
| N(21) | 8977(6) | 3765(3) | 5366(3) | 32(1) |
| N(22) | 5331(5) | 3025(2) | 6005(3) | 24(1) |
| N(23) | 1281(6) | 3535(2) | 3319(3) | 27(1) |
| N(24) | 5003(6) | 4316(2) | 2726(3) | 26(1) |
| Pt(3) | 5000 | 0 | 0 | 18(1) |
| C(31) | 3419(6) | 361(2) | 337(3) | 21(1) |
| N(31) | 2503(6) | 572(2) | 520(3) | 26(1) |
| C(32) | 6865(7) | 225(3) | 1155(3) | 24(1) |
| N(32) | 7944(7) | 356(3) | 1824(3) | 36(1) |
| Pt(4) | 5000 | 0 | 5000 | 55(1) |
| C(41) | 3207(11) | -32(6) | 3816(5) | 68(3) |
| N(41) | 2173(12) | -45(8) | 3121(5) | 119(6) |
| C(42) | 6669(11) | 121(6) | 4613(5) | 70(3) |
| N(42) | 7618(11) | 188(6) | 4381(5) | 97(4) |

| | x | y | z | U(eq) | sof |
|---|---|---|---|---|---|
| O(1) | 1697(10) | 1036(4) | 2063(5) | 49(3) | 0.687 |
| O(2) | 9630(15) | 1009(7) | 3401(10) | 53(4) | 0.471 |
| O(2A) | -560(30) | 1086(12) | 3790(20) | 53(4) | 0.282 |
| O(3) | 650(20) | 1338(7) | 5006(17) | 104(8) | 0.680 |
| O(3A) | -80(140) | 1160(40) | 4480(110) | 104(8) | 0.129 |
| Cs(1) | 5355(4) | 911(1) | 2458(2) | 30(1) | 0.847 |
| Cs(1A) | 5621(13) | 850(4) | 2642(8) | 30(1) | 0.153 |
| Cs(2) | 9496(1) | 2198(1) | 2146(1) | 30(1) | 0.746 |
| Cs(2A) | 9525(2) | 1852(1) | 2191(1) | 30(1) | 0.254 |
| Cs(3) | 1234(3) | 2854(2) | 4999(1) | 24(1) | 0.863 |
| Cs(3A) | 1068(11) | 2715(7) | 4967(4) | 24(1) | 0.137 |
| Cs(4) | 811(1) | 4247(1) | 1543(1) | 34(1) | 0.741 |
| Cs(4A) | 598(2) | 4511(1) | 1592(1) | 34(1) | 0.129 |
| Cs(5) | 9088(1) | 4473(1) | 3736(1) | 26(1) | 0.609 |
| Cs(5A) | 9309(2) | 4715(1) | 3763(1) | 26(1) | 0.391 |
| Cs(6) | 5298(3) | 3477(1) | 1321(1) | 35(1) | 0.677 |
| Cs(6A) | 4799(5) | 3483(2) | 1228(2) | 35(1) | 0.323 |

Table 3. Bond lengths [Å] and angles [°] for $Cs_2Pt(CN)_4*0.75H_2O$.

| | | | |
|---|---|---|---|
| Pt(1)-C(11) | 2.007(6) | C(13)-Pt(1)-C(14) | 87.0(2) |
| Pt(1)-C(12) | 2.007(6) | C(12)-Pt(1)-C(11) | 88.9(3) |
| Pt(1)-C(13) | 2.000(7) | C(14)-Pt(1)-C(11) | 91.1(2) |
| Pt(1)-C(14) | 2.007(6) | C(13)-Pt(1)-C(12) | 92.9(3) |
| C(11)-N(11) | 1.154(9) | C(13)-Pt(1)-C(11) | 177.8(2) |
| C(12)-N(12) | 1.153(9) | C(14)-Pt(1)-C(12) | 179.5(2) |
| C(13)-N(13) | 1.166(9) | | |
| C(14)-N(14) | 1.163(8) | C(21)-Pt(2)-C(22) | 88.6(2) |
| Pt(2)-C(21) | 1.996(5) | C(24)-Pt(2)-C(23) | 89.2(2) |
| Pt(2)-C(22) | 2.010(5) | C(21)-Pt(2)-C(24) | 90.7(2) |
| Pt(2)-C(23) | 2.013(5) | C(22)-Pt(2)-C(23) | 91.5(2) |
| Pt(2)-C(24) | 2.004(5) | C(24)-Pt(2)-C(22) | 178.8(2) |
| C(21)-N(21) | 1.160(7) | C(21)-Pt(2)-C(23) | 179.9(2) |
| C(22)-N(22) | 1.157(7) | | |
| C(23)-N(23) | 1.158(7) | C(32)-Pt(3)-C(31) | 89.8(2) (2x) |
| C(24)-N(24) | 1.167(7) | C(32)-Pt(3)-C(31) | 90.2(2) (2x) |
| Pt(3)-C(31) | 2.006(5) (2x) | C(31)-Pt(3)-C(31) | 180.0 (2x) |
| Pt(3)-C(32) | 2.005(6) (2x) | | |
| C(31)-N(31) | 1.151(7) | C(41)-Pt(4)-C(42) | 88.2(4) (2x) |
| C(32)-N(32) | 1.161(8) | C(41)-Pt(4)-C(42) | 91.8(4) (2x) |
| Pt(4)-C(41) | 1.960(8) (2x) | C(42)-Pt(4)-C(42) | 180.0 (2x) |
| Pt(4)-C(42) | 2.021(12) (2x) | | |
| C(41)-N(41) | 1.145(11) | Pt(2)-Pt(3)-Pt(2) | 180.0 |
| C(42)-N(42) | 1.163(15) | Pt(1)-Pt(2)-Pt(3) | 178.779(1) |
| Pt(1)-Pt(2) | 3.1402(3) | | |
| Pt(2)-Pt(3) | 3.0880(2) (2x) | | |

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cs_2Pt(CN)_4*H_2O$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Pt(1) | 19(1) | 24(1) | 24(1) | -8(1) | 7(1) | 3(1) |
| C(11) | 27(2) | 27(3) | 33(3) | -3(2) | 9(2) | 1(2) |
| C(12) | 30(3) | 32(3) | 36(3) | -3(2) | 14(2) | 8(2) |
| C(13) | 24(2) | 50(4) | 23(2) | -15(2) | 9(2) | 0(2) |
| C(14) | 25(2) | 39(3) | 25(2) | -12(2) | 12(2) | -1(2) |
| N(11) | 36(3) | 38(3) | 50(3) | 4(2) | 19(3) | -1(2) |
| N(12) | 43(3) | 53(4) | 36(3) | 2(3) | 8(3) | 19(3) |
| N(13) | 25(2) | 88(5) | 32(3) | -7(3) | 12(2) | -1(3) |
| N(14) | 25(2) | 70(4) | 24(2) | -8(2) | 10(2) | 6(2) |
| Pt(2) | 17(1) | 17(1) | 18(1) | -2(1) | 10(1) | 1(1) |
| C(21) | 22(2) | 28(2) | 22(2) | -2(2) | 14(2) | 3(2) |
| C(22) | 17(2) | 18(2) | 24(2) | -2(2) | 9(2) | 2(2) |
| C(23) | 24(2) | 23(2) | 16(2) | 0(2) | 11(2) | 1(2) |
| C(24) | 18(2) | 24(2) | 19(2) | -4(2) | 10(2) | 0(2) |
| N(21) | 22(2) | 49(3) | 27(2) | -4(2) | 15(2) | 4(2) |
| N(22) | 21(2) | 28(2) | 25(2) | 2(2) | 12(2) | 1(2) |
| N(23) | 27(2) | 35(2) | 24(2) | -2(2) | 16(2) | -1(2) |
| N(24) | 30(2) | 28(2) | 23(2) | -4(2) | 14(2) | 0(2) |
| Pt(3) | 21(1) | 17(1) | 22(1) | 5(1) | 15(1) | 3(1) |
| C(31) | 22(2) | 23(2) | 22(2) | 5(2) | 14(2) | 5(2) |
| N(31) | 29(2) | 28(2) | 28(2) | 3(2) | 18(2) | 3(2) |
| C(32) | 30(2) | 25(2) | 28(2) | 5(2) | 22(2) | 2(2) |
| N(32) | 34(3) | 38(3) | 33(3) | 1(2) | 17(2) | 0(2) |
| Pt(4) | 38(1) | 68(1) | 33(1) | -30(1) | -3(1) | 21(1) |
| C(41) | 49(5) | 101(8) | 35(4) | -13(4) | 6(3) | 30(5) |
| N(41) | 55(5) | 238(16) | 35(4) | -29(6) | 1(4) | 60(7) |
| C(42) | 46(4) | 103(8) | 35(4) | -32(4) | 1(3) | 26(5) |
| N(42) | 59(5) | 166(11) | 39(4) | -35(5) | 5(4) | 34(6) |
| O(1) | 46(4) | 61(5) | 39(4) | 1(3) | 21(3) | 13(4) |
| O(2) | 38(5) | 62(7) | 59(9) | -7(6) | 23(5) | -6(4) |
| O(2A) | 38(5) | 62(7) | 59(9) | -7(6) | 23(5) | -6(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(3) | 75(11) | 61(8) | 180(20) | 27(10) | 62(13) | -11(7) |
| O(3A) | 75(11) | 61(8) | 180(20) | 27(10) | 62(13) | -11(7) |
| Cs(1) | 43(1) | 25(1) | 25(1) | -4(1) | 19(1) | 3(1) |
| Cs(1A) | 43(1) | 25(1) | 25(1) | -4(1) | 19(1) | 3(1) |
| Cs(2) | 21(1) | 45(1) | 25(1) | -5(1) | 12(1) | 1(1) |
| Cs(2A) | 21(1) | 45(1) | 25(1) | -5(1) | 12(1) | 1(1) |
| Cs(3) | 20(1) | 32(1) | 20(1) | 2(1) | 10(1) | 4(1) |
| Cs(3A) | 20(1) | 32(1) | 20(1) | 2(1) | 10(1) | 4(1) |
| Cs(4) | 26(1) | 45(1) | 28(1) | -4(1) | 13(1) | -7(1) |
| Cs(4A) | 26(1) | 45(1) | 28(1) | -4(1) | 13(1) | -7(1) |
| Cs(5) | 24(1) | 33(1) | 22(1) | 3(1) | 12(1) | 10(1) |
| Cs(5A) | 24(1) | 33(1) | 22(1) | 3(1) | 12(1) | 10(1) |
| Cs(6) | 55(1) | 28(1) | 36(1) | -10(1) | 34(1) | -12(1) |
| Cs(6A) | 55(1) | 28(1) | 36(1) | -10(1) | 34(1) | -12(1) |

```
data_Cs2Pt(CN)4.nH2O

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C4 H1.5 Cs2 N4 O0.75 Pt'
_chemical_formula_weight          592.004

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cs'  'Cs'  -0.3680   2.1192
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Pt'  'Pt'  -1.7033   8.3905
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            'monoclinic'
_symmetry_space_group_name_H-M    'P 21/c'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

_cell_length_a                    9.40820(10)
_cell_length_b                    20.8216(4)
_cell_length_c                    17.9431(3)
_cell_angle_alpha                 90.00
_cell_angle_beta                  119.410(2)
_cell_angle_gamma                 90.00
_cell_volume                      3061.96(8)
_cell_formula_units_Z             12
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     56894
_cell_measurement_theta_min       1.63
_cell_measurement_theta_max       30.51

_exptl_crystal_description        'platelet'
_exptl_crystal_colour             'orange'
```

```
_exptl_crystal_size_max           0.16
_exptl_crystal_size_mid           0.05
_exptl_crystal_size_min           0.01
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     3.755
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2952
_exptl_absorpt_coefficient_mu     20.735
_exptl_absorpt_correction_type    'analytical'
_exptl_absorpt_correction_T_min   ?
_exptl_absorpt_correction_T_max   ?
_exptl_absorpt_process_details    'SADABS'

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       100(2)
_diffrn_radiation_wavelength      0.70000
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             56894
_diffrn_reflns_av_R_equivalents   0.0406
_diffrn_reflns_av_sigmaI/netI     0.0266
_diffrn_reflns_limit_h_min        -13
_diffrn_reflns_limit_h_max        13
_diffrn_reflns_limit_k_min        -29
_diffrn_reflns_limit_k_max        29
_diffrn_reflns_limit_l_min        -24
_diffrn_reflns_limit_l_max        25
_diffrn_reflns_theta_min          1.63
_diffrn_reflns_theta_max          30.51
_reflns_number_total              9340
_reflns_number_gt                 8357
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        ?
_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
```

```
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0366P)^2^+19.0900P] where
P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    ?
_refine_ls_hydrogen_treatment     ?
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          9340
_refine_ls_number_parameters      363
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0326
_refine_ls_R_factor_gt            0.0290
_refine_ls_wR_factor_ref          0.0745
_refine_ls_wR_factor_gt           0.0728
_refine_ls_goodness_of_fit_ref    1.034
_refine_ls_restrained_S_all       1.034
_refine_ls_shift/su_max           0.002
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Pt1 Pt 0.53196(2) 0.225215(10) 0.371918(13) 0.02371(5) Uani 1 1 d . . .
C11 C 0.3632(7) 0.1921(3) 0.3998(4) 0.0312(11) Uani 1 1 d . . .
C12 C 0.7059(7) 0.1979(3) 0.4887(4) 0.0339(12) Uani 1 1 d . . .
C13 C 0.6946(7) 0.2571(3) 0.3394(4) 0.0335(13) Uani 1 1 d . . .
C14 C 0.3583(7) 0.2518(3) 0.2547(4) 0.0295(11) Uani 1 1 d . . .
N11 N 0.2686(7) 0.1730(3) 0.4176(4) 0.0423(13) Uani 1 1 d . . .
```

```
N12 N 0.8011(8) 0.1822(3) 0.5569(4) 0.0487(15) Uani 1 1 d . . .
N13 N 0.7830(7) 0.2782(4) 0.3176(4) 0.0489(16) Uani 1 1 d . . .
N14 N 0.2620(6) 0.2696(3) 0.1870(3) 0.0405(13) Uani 1 1 d . . .
Pt2 Pt 0.51388(2) 0.364279(8) 0.434489(11) 0.01667(4) Uani 1 1 d . . .
C21 C 0.7568(6) 0.3713(3) 0.4984(3) 0.0228(9) Uani 1 1 d . . .
C22 C 0.5246(6) 0.3244(2) 0.5391(3) 0.0204(8) Uani 1 1 d . . .
C23 C 0.2690(6) 0.3570(2) 0.3698(3) 0.0203(8) Uani 1 1 d . . .
C24 C 0.5057(6) 0.4057(2) 0.3316(3) 0.0202(8) Uani 1 1 d . . .
N21 N 0.8977(6) 0.3765(3) 0.5366(3) 0.0317(10) Uani 1 1 d . . .
N22 N 0.5331(5) 0.3025(2) 0.6005(3) 0.0241(8) Uani 1 1 d . . .
N23 N 0.1281(6) 0.3535(2) 0.3319(3) 0.0274(9) Uani 1 1 d . . .
N24 N 0.5003(6) 0.4316(2) 0.2726(3) 0.0264(9) Uani 1 1 d . . .
Pt3 Pt 0.5000 0.0000 0.0000 0.01798(5) Uani 1 2 d S . .
C31 C 0.3419(6) 0.0361(2) 0.0337(3) 0.0208(9) Uani 1 1 d . . .
N31 N 0.2503(6) 0.0572(2) 0.0520(3) 0.0263(9) Uani 1 1 d . . .
C32 C 0.6865(7) 0.0225(3) 0.1155(3) 0.0244(9) Uani 1 1 d . . .
N32 N 0.7944(7) 0.0356(3) 0.1824(3) 0.0355(11) Uani 1 1 d . . .
Pt4 Pt 0.5000 0.0000 0.5000 0.05520(14) Uani 1 2 d S . .
C41 C 0.3207(11) -0.0032(6) 0.3816(5) 0.068(3) Uani 1 1 d . . .
N41 N 0.2173(12) -0.0045(8) 0.3121(5) 0.119(6) Uani 1 1 d . . .
C42 C 0.6669(11) 0.0121(6) 0.4613(5) 0.070(3) Uani 1 1 d . . .
N42 N 0.7618(11) 0.0188(6) 0.4381(5) 0.097(4) Uani 1 1 d . . .
O1 O 0.1697(10) 0.1036(4) 0.2063(5) 0.049(3) Uani 0.687(19) 1 d P . .
O2 O 0.9630(15) 0.1009(7) 0.3401(10) 0.053(4) Uani 0.47(2) 1 d P . .
O2A O -0.056(3) 0.1086(12) 0.379(2) 0.053(4) Uani 0.282(18) 1 d P . .
O3 O 0.065(2) 0.1338(7) 0.5006(17) 0.104(8) Uani 0.68(4) 1 d P . .
O3A O -0.008(14) 0.116(4) 0.448(11) 0.104(8) Uani 0.13(3) 1 d P . .
Cs1 Cs 0.5355(4) 0.09106(9) 0.2458(2) 0.0303(3) Uani 0.847(17) 1 d P .
.
Cs1A Cs 0.5621(13) 0.0850(4) 0.2642(8) 0.0303(3) Uani 0.153(17) 1 d P .
.
Cs2 Cs 0.94958(6) 0.21979(3) 0.21461(3) 0.03041(12) Uani 0.7465(11) 1 d
P . .
Cs2A Cs 0.95248(17) 0.18515(10) 0.21908(9) 0.03041(12) Uani 0.2535(11)
1 d P . .
Cs3 Cs 0.1234(3) 0.2854(2) 0.49986(7) 0.0239(3) Uani 0.863(19) 1 d P .
.
Cs3A Cs 0.1068(11) 0.2715(7) 0.4967(4) 0.0239(3) Uani 0.137(19) 1 d P .
.
Cs4 Cs 0.08115(7) 0.42471(4) 0.15435(4) 0.03355(15) Uani 0.7414(18) 1 d
P . .
Cs4A Cs 0.0598(2) 0.45107(13) 0.15919(12) 0.03355(15) Uani 0.2586(18) 1
d P . .
Cs5 Cs 0.90884(10) 0.44734(5) 0.37361(5) 0.02587(15) Uani 0.6090(16) 1
d P . .
Cs5A Cs 0.93091(17) 0.47154(7) 0.37627(9) 0.02587(15) Uani 0.3910(16) 1
d P . .
Cs6 Cs 0.5298(3) 0.34765(7) 0.13212(11) 0.0345(3) Uani 0.677(6) 1 d P .
.
Cs6A Cs 0.4799(5) 0.34835(16) 0.1228(2) 0.0345(3) Uani 0.323(6) 1 d P .
.

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
```

```
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Pt1 0.01899(8) 0.02393(9) 0.02365(9) -0.00798(6) 0.00694(7) 0.00293(6)
C11 0.027(2) 0.027(3) 0.033(3) -0.003(2) 0.009(2) 0.001(2)
C12 0.030(3) 0.032(3) 0.036(3) -0.003(2) 0.014(2) 0.008(2)
C13 0.024(2) 0.050(4) 0.023(2) -0.015(2) 0.009(2) 0.000(2)
C14 0.025(2) 0.039(3) 0.025(2) -0.012(2) 0.012(2) -0.001(2)
N11 0.036(3) 0.038(3) 0.050(3) 0.004(2) 0.019(3) -0.001(2)
N12 0.043(3) 0.053(4) 0.036(3) 0.002(3) 0.008(3) 0.019(3)
N13 0.025(2) 0.088(5) 0.032(3) -0.007(3) 0.012(2) -0.001(3)
N14 0.025(2) 0.070(4) 0.024(2) -0.008(2) 0.010(2) 0.006(2)
Pt2 0.01701(8) 0.01740(8) 0.01762(8) -0.00203(5) 0.01006(6) 0.00123(5)
C21 0.022(2) 0.028(2) 0.022(2) -0.0021(17) 0.0143(19) 0.0031(18)
C22 0.0174(19) 0.018(2) 0.024(2) -0.0016(16) 0.0086(17) 0.0015(15)
C23 0.024(2) 0.023(2) 0.0160(19) -0.0001(15) 0.0114(17) 0.0010(17)
C24 0.0184(19) 0.024(2) 0.019(2) -0.0043(16) 0.0104(16) 0.0001(16)
N21 0.022(2) 0.049(3) 0.027(2) -0.004(2) 0.0148(18) 0.0040(19)
N22 0.0208(19) 0.028(2) 0.025(2) 0.0019(16) 0.0124(16) 0.0008(16)
N23 0.027(2) 0.035(2) 0.024(2) -0.0021(17) 0.0155(18) -0.0014(18)
N24 0.030(2) 0.028(2) 0.023(2) -0.0035(16) 0.0145(18) -0.0002(17)
Pt3 0.02129(11) 0.01665(11) 0.02182(11) 0.00450(8) 0.01507(9)
0.00297(8)
C31 0.022(2) 0.023(2) 0.022(2) 0.0054(16) 0.0143(18) 0.0052(17)
N31 0.029(2) 0.028(2) 0.028(2) 0.0032(17) 0.0183(18) 0.0030(17)
C32 0.030(2) 0.025(2) 0.028(2) 0.0046(18) 0.022(2) 0.0018(19)
N32 0.034(3) 0.038(3) 0.033(3) 0.001(2) 0.017(2) 0.000(2)
Pt4 0.03818(19) 0.0679(3) 0.03261(18) -0.02989(18) -0.00338(15)
0.02119(18)
C41 0.049(5) 0.101(8) 0.035(4) -0.013(4) 0.006(3) 0.030(5)
N41 0.055(5) 0.238(16) 0.035(4) -0.029(6) 0.001(4) 0.060(7)
C42 0.046(4) 0.103(8) 0.035(4) -0.032(4) 0.001(3) 0.026(5)
N42 0.059(5) 0.166(11) 0.039(4) -0.035(5) 0.005(4) 0.034(6)
O1 0.046(4) 0.061(5) 0.039(4) 0.001(3) 0.021(3) 0.013(4)
O2 0.038(5) 0.062(7) 0.059(9) -0.007(6) 0.023(5) -0.006(4)
O2A 0.038(5) 0.062(7) 0.059(9) -0.007(6) 0.023(5) -0.006(4)
O3 0.075(11) 0.061(8) 0.18(2) 0.027(10) 0.062(13) -0.011(7)
O3A 0.075(11) 0.061(8) 0.18(2) 0.027(10) 0.062(13) -0.011(7)
Cs1 0.0433(5) 0.0249(3) 0.0249(7) -0.0043(4) 0.0185(6) 0.0026(3)
Cs1A 0.0433(5) 0.0249(3) 0.0249(7) -0.0043(4) 0.0185(6) 0.0026(3)
Cs2 0.02123(17) 0.0455(3) 0.02500(18) -0.0054(2) 0.01173(14) 0.0010(2)
Cs2A 0.02123(17) 0.0455(3) 0.02500(18) -0.0054(2) 0.01173(14) 0.0010(2)
Cs3 0.0196(3) 0.0315(8) 0.02022(15) 0.0022(3) 0.00959(17) 0.0041(4)
Cs3A 0.0196(3) 0.0315(8) 0.02022(15) 0.0022(3) 0.00959(17) 0.0041(4)
Cs4 0.0261(2) 0.0452(4) 0.02838(19) -0.0042(3) 0.01258(16) -0.0074(3)
Cs4A 0.0261(2) 0.0452(4) 0.02838(19) -0.0042(3) 0.01258(16) -0.0074(3)
Cs5 0.0239(3) 0.0334(5) 0.02177(16) 0.0029(3) 0.01228(18) 0.0098(3)
Cs5A 0.0239(3) 0.0334(5) 0.02177(16) 0.0029(3) 0.01228(18) 0.0098(3)
Cs6 0.0550(9) 0.02812(19) 0.0355(4) -0.0104(2) 0.0339(6) -0.0123(5)
Cs6A 0.0550(9) 0.02812(19) 0.0355(4) -0.0104(2) 0.0339(6) -0.0123(5)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
```

```
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
Pt1 C13 2.000(7) . ?
Pt1 C14 2.007(6) . ?
Pt1 C12 2.007(6) . ?
Pt1 C11 2.007(6) . ?
Pt1 Pt2 3.1402(3) . ?
Pt1 Cs1A 3.589(6) . ?
Pt1 Cs1 3.6052(10) . ?
C11 N11 1.154(9) . ?
C11 Cs2A 3.628(6) 1_455 ?
C11 Cs6A 3.690(7) 4_566 ?
C11 Cs2 3.717(6) 1_455 ?
C11 Cs6 3.755(6) 4_566 ?
C12 N12 1.153(9) . ?
C12 Cs6 3.801(7) 4_566 ?
C13 N13 1.166(9) . ?
C13 Cs3A 3.514(11) 1_655 ?
C13 Cs3 3.675(6) 1_655 ?
C13 Cs6 3.759(7) . ?
C13 Cs1 3.813(6) . ?
C13 Cs1A 3.816(9) . ?
C13 Cs6A 3.883(8) . ?
C14 N14 1.163(8) . ?
C14 Cs2 3.610(6) 1_455 ?
C14 Cs6A 3.688(7) . ?
C14 Cs1 3.778(6) . ?
C14 Cs2A 3.810(6) 1_455 ?
C14 Cs6 3.861(7) . ?
N11 Cs6A 3.243(7) 4_566 ?
N11 Cs3A 3.265(11) . ?
N11 Cs2A 3.346(6) 1_455 ?
N11 Cs3 3.391(7) . ?
N11 Cs6 3.427(7) 4_566 ?
N11 Cs2 3.534(6) 1_455 ?
N12 Cs2 3.200(7) 4_566 ?
N12 Cs4 3.229(6) 4_666 ?
N12 Cs6 3.478(8) 4_566 ?
N12 Cs4A 3.549(6) 4_666 ?
N12 Cs2A 3.749(7) 4_566 ?
N12 Cs6A 3.800(8) 4_566 ?
N13 Cs3A 3.165(10) 1_655 ?
N13 Cs2 3.193(6) . ?
```

```
N13 Cs3 3.269(6) 1_655 ?
N13 Cs6 3.324(7) . ?
N13 Cs2A 3.491(7) . ?
N13 Cs6A 3.562(8) . ?
N13 Cs5 3.693(8) . ?
N14 Cs3A 3.102(8) 4_565 ?
N14 Cs3 3.160(5) 4_565 ?
N14 Cs6A 3.245(7) . ?
N14 Cs2 3.375(6) 1_455 ?
N14 Cs6 3.521(7) . ?
N14 Cs4 3.562(7) . ?
N14 Cs2A 3.681(7) 1_455 ?
Pt2 C21 1.996(5) . ?
Pt2 C24 2.004(5) . ?
Pt2 C22 2.010(5) . ?
Pt2 C23 2.013(5) . ?
Pt2 Pt3 3.08795(17) 2_655 ?
C21 N21 1.160(7) . ?
C21 Cs5 3.566(5) . ?
C21 Cs2A 3.645(5) 4_566 ?
C21 Cs3 3.874(5) 1_655 ?
C21 Cs2 3.876(5) 4_566 ?
C21 Cs3A 3.907(8) 1_655 ?
C22 N22 1.157(7) . ?
C22 Cs3 3.576(6) . ?
C22 Cs2A 3.729(5) 4_566 ?
C22 Cs3A 3.782(13) . ?
C22 Cs2 3.792(5) 4_566 ?
C23 N23 1.158(7) . ?
C23 Cs3 3.561(6) . ?
C23 Cs4 3.653(5) . ?
C23 Cs3A 3.754(12) . ?
C23 Cs4A 3.832(5) . ?
C23 Cs5 3.905(5) 1_455 ?
C24 N24 1.167(7) . ?
C24 Cs5 3.591(5) . ?
C24 Cs4 3.708(5) . ?
C24 Cs6A 3.825(6) . ?
C24 Cs6 3.890(5) . ?
C24 Cs4A 3.914(5) . ?
N21 Cs3 3.149(5) 1_655 ?
N21 Cs3A 3.247(10) 1_655 ?
N21 Cs2A 3.314(5) 4_566 ?
N21 Cs5 3.322(5) . ?
N21 Cs5A 3.546(6) 3_766 ?
N21 Cs2 3.596(5) 4_566 ?
N21 Cs5A 3.629(6) . ?
N22 Cs6 3.180(5) 4_566 ?
N22 Cs6A 3.236(6) 4_566 ?
N22 Cs3 3.378(5) . ?
N22 Cs1 3.415(6) 4_566 ?
N22 Cs2 3.447(4) 4_566 ?
N22 Cs2A 3.452(5) 4_566 ?
N22 Cs3A 3.554(12) . ?
N22 Cs1A 3.662(12) 4_566 ?
N23 Cs5 3.186(5) 1_455 ?
N23 Cs4 3.341(5) . ?
```

```
N23 Cs3 3.350(5) . ?
N23 Cs2 3.396(5) 1_455 ?
N23 Cs5A 3.401(5) 1_455 ?
N23 Cs4A 3.491(5) . ?
N23 Cs3A 3.505(11) . ?
N24 Cs6A 3.124(5) . ?
N24 Cs6 3.191(5) . ?
N24 Cs1A 3.255(8) 2_655 ?
N24 Cs1 3.336(5) 2_655 ?
N24 Cs5 3.365(5) . ?
N24 Cs4 3.443(5) . ?
N24 Cs5A 3.628(5) . ?
N24 Cs4A 3.633(5) . ?
Pt3 C32 2.005(6) . ?
Pt3 C32 2.005(6) 3_655 ?
Pt3 C31 2.006(5) . ?
Pt3 C31 2.006(5) 3_655 ?
Pt3 Pt2 3.08794(17) 4_565 ?
Pt3 Pt2 3.08795(17) 2_645 ?
C31 N31 1.151(7) . ?
C31 Cs5A 3.497(5) 4_465 ?
C31 Cs1 3.509(6) . ?
C31 Cs5 3.671(5) 4_465 ?
C31 Cs1A 3.745(12) . ?
C31 Cs5A 3.884(5) 2_645 ?
N31 Cs5A 3.145(5) 2_645 ?
N31 Cs5A 3.166(5) 4_465 ?
N31 Cs5 3.237(5) 4_465 ?
N31 Cs1 3.259(6) . ?
N31 Cs5 3.348(5) 2_645 ?
N31 Cs3 3.456(7) 4_565 ?
N31 Cs1A 3.531(13) . ?
N31 Cs3A 3.770(17) 4_565 ?
C32 N32 1.161(8) . ?
C32 Cs1 3.577(5) . ?
C32 Cs1A 3.640(8) . ?
C32 Cs5A 3.685(5) 2_745 ?
C32 Cs4A 3.844(6) 2_645 ?
N32 Cs4A 3.038(6) 2_645 ?
N32 Cs1A 3.338(8) . ?
N32 Cs1 3.360(6) . ?
N32 Cs2A 3.374(6) . ?
N32 Cs4 3.451(6) 2_645 ?
N32 Cs5A 3.497(6) 2_745 ?
Pt4 C41 1.960(8) 3_656 ?
Pt4 C41 1.960(8) . ?
Pt4 C42 2.021(12) . ?
Pt4 C42 2.021(12) 3_656 ?
Pt4 Cs6 3.8868(14) 4_566 ?
Pt4 Cs6 3.8868(14) 2_645 ?
Pt4 Cs6A 3.908(3) 4_566 ?
Pt4 Cs6A 3.908(3) 2_645 ?
C41 N41 1.145(11) . ?
C41 Cs4A 3.418(11) 2_545 ?
C41 Cs6 3.468(10) 2_645 ?
C41 Cs6A 3.638(10) 2_645 ?
C41 Cs4 3.817(12) 2_545 ?
```

```
N41 Cs5A 2.999(8) 2_645 ?
N41 Cs4A 3.039(14) 2_545 ?
N41 Cs5 3.105(8) 2_645 ?
N41 Cs4 3.476(15) 2_545 ?
N41 Cs6 3.715(12) 2_645 ?
C42 N42 1.163(15) . ?
C42 Cs1A 3.515(16) . ?
C42 Cs6A 3.711(11) 2_645 ?
C42 Cs4A 3.738(8) 4_666 ?
C42 Cs1 3.805(12) . ?
C42 Cs6 3.862(11) 2_645 ?
N42 Cs1A 3.068(17) . ?
N42 Cs4A 3.277(9) 2_645 ?
N42 Cs4 3.344(9) 2_645 ?
N42 Cs1 3.390(11) . ?
N42 Cs4A 3.614(8) 4_666 ?
N42 Cs4 3.743(8) 4_666 ?
O1 Cs2A 2.752(8) 1_455 ?
O1 Cs5A 3.045(9) 2_645 ?
O1 Cs1 3.165(8) . ?
O1 Cs2 3.236(8) 1_455 ?
O1 Cs1A 3.331(12) . ?
O1 Cs5 3.484(9) 2_645 ?
O2 O2A 0.81(3) 1_655 ?
O2 Cs2A 2.755(15) . ?
O2 Cs4A 3.127(15) 2_645 ?
O2 Cs2 3.307(15) . ?
O2 Cs1A 3.339(16) . ?
O2 Cs1 3.522(13) . ?
O2 Cs4 3.699(14) 2_645 ?
O2A O2 0.81(3) 1_455 ?
O2A O3A 1.11(16) . ?
O2A Cs1A 3.18(2) 1_455 ?
O2A Cs2A 3.31(3) 1_455 ?
O2A Cs4A 3.35(3) 2_545 ?
O2A Cs1 3.40(2) 1_455 ?
O2A Cs2 3.77(3) 1_455 ?
O3 O3A 0.93(16) . ?
O3 Cs3A 2.90(2) . ?
O3 Cs4 2.949(19) 4_566 ?
O3 Cs3 3.206(16) . ?
O3 Cs4A 3.369(17) 4_566 ?
O3 Cs6A 3.43(2) 4_566 ?
O3A Cs3A 3.40(11) . ?
O3A Cs4 3.47(15) 4_566 ?
O3A Cs3 3.71(11) . ?
O3A Cs4A 3.78(14) 4_566 ?
Cs1 N24 3.336(5) 2_645 ?
Cs1 O2A 3.40(2) 1_655 ?
Cs1 N22 3.415(6) 4_565 ?
Cs1A O2A 3.18(2) 1_655 ?
Cs1A N24 3.255(8) 2_645 ?
Cs1A N22 3.662(12) 4_565 ?
Cs2 Cs2A 0.7247(19) . ?
Cs2 N12 3.200(7) 4_565 ?
Cs2 O1 3.236(8) 1_655 ?
Cs2 N14 3.375(6) 1_655 ?
```

```
Cs2 N23 3.396(5) 1_655 ?
Cs2 N22 3.447(4) 4_565 ?
Cs2 N11 3.534(6) 1_655 ?
Cs2 N21 3.596(5) 4_565 ?
Cs2 C14 3.610(6) 1_655 ?
Cs2 C11 3.717(6) 1_655 ?
Cs2A O1 2.752(8) 1_655 ?
Cs2A O2A 3.31(3) 1_655 ?
Cs2A N21 3.314(5) 4_565 ?
Cs2A N11 3.346(6) 1_655 ?
Cs2A N22 3.452(5) 4_565 ?
Cs2A C11 3.628(6) 1_655 ?
Cs2A C21 3.645(5) 4_565 ?
Cs2A N14 3.681(7) 1_655 ?
Cs3 N21 3.149(5) 1_455 ?
Cs3 N14 3.160(5) 4_566 ?
Cs3 N13 3.269(6) 1_455 ?
Cs3 N31 3.456(7) 4_566 ?
Cs3 C13 3.675(6) 1_455 ?
Cs3A N14 3.102(8) 4_566 ?
Cs3A N13 3.165(10) 1_455 ?
Cs3A N21 3.247(10) 1_455 ?
Cs3A C13 3.514(11) 1_455 ?
Cs3A N31 3.770(17) 4_566 ?
Cs4 Cs4A 0.605(2) . ?
Cs4 O3 2.949(19) 4_565 ?
Cs4 N12 3.229(6) 4_465 ?
Cs4 N42 3.344(9) 2_655 ?
Cs4 N32 3.451(6) 2_655 ?
Cs4 O3A 3.47(15) 4_565 ?
Cs4 N41 3.476(15) 2 ?
Cs4 O2 3.699(14) 2_655 ?
Cs4A N32 3.038(6) 2_655 ?
Cs4A N41 3.039(14) 2 ?
Cs4A O2 3.127(15) 2_655 ?
Cs4A N42 3.277(9) 2_655 ?
Cs4A O2A 3.35(3) 2 ?
Cs4A O3 3.369(17) 4_565 ?
Cs4A C41 3.418(11) 2 ?
Cs4A N12 3.549(6) 4_465 ?
Cs4A N42 3.614(8) 4_465 ?
Cs5 Cs5A 0.5381(11) . ?
Cs5 N41 3.105(8) 2_655 ?
Cs5 N23 3.186(5) 1_655 ?
Cs5 N31 3.237(5) 4_666 ?
Cs5 N31 3.348(5) 2_655 ?
Cs5 O1 3.484(9) 2_655 ?
Cs5 C31 3.671(5) 4_666 ?
Cs5A N41 2.999(8) 2_655 ?
Cs5A O1 3.045(9) 2_655 ?
Cs5A N31 3.145(5) 2_655 ?
Cs5A N31 3.166(5) 4_666 ?
Cs5A N23 3.401(5) 1_655 ?
Cs5A C31 3.497(5) 4_666 ?
Cs5A N32 3.497(6) 2_755 ?
Cs5A N21 3.546(6) 3_766 ?
Cs5A C32 3.685(5) 2_755 ?
```

```
Cs6 N22 3.180(5) 4_565 ?
Cs6 N11 3.427(7) 4_565 ?
Cs6 C41 3.468(10) 2_655 ?
Cs6 N12 3.478(8) 4_565 ?
Cs6 N41 3.715(12) 2_655 ?
Cs6 C11 3.755(6) 4_565 ?
Cs6 C12 3.801(7) 4_565 ?
Cs6A N22 3.236(6) 4_565 ?
Cs6A N11 3.243(7) 4_565 ?
Cs6A O3 3.43(2) 4_565 ?
Cs6A C41 3.638(10) 2_655 ?
Cs6A C11 3.690(7) 4_565 ?
Cs6A C42 3.711(11) 2_655 ?
Cs6A N12 3.800(8) 4_565 ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
C13 Pt1 C14 87.0(2) . . ?
C13 Pt1 C12 92.9(3) . . ?
C14 Pt1 C12 179.5(2) . . ?
C13 Pt1 C11 177.8(2) . . ?
C14 Pt1 C11 91.1(2) . . ?
C12 Pt1 C11 88.9(3) . . ?
C13 Pt1 Pt2 88.97(18) . . ?
C14 Pt1 Pt2 87.76(16) . . ?
C12 Pt1 Pt2 92.73(17) . . ?
C11 Pt1 Pt2 92.25(17) . . ?
C13 Pt1 Cs1A 80.7(2) . . ?
C14 Pt1 Cs1A 84.2(3) . . ?
C12 Pt1 Cs1A 95.3(3) . . ?
C11 Pt1 Cs1A 97.8(2) . . ?
Pt2 Pt1 Cs1A 167.21(16) . . ?
C13 Pt1 Cs1 80.19(17) . . ?
C14 Pt1 Cs1 79.03(17) . . ?
C12 Pt1 Cs1 100.47(18) . . ?
C11 Pt1 Cs1 98.19(17) . . ?
Pt2 Pt1 Cs1 163.26(6) . . ?
Cs1A Pt1 Cs1 5.19(16) . . ?
N11 C11 Pt1 178.6(6) . . ?
N11 C11 Cs2A 66.8(4) . 1_455 ?
Pt1 C11 Cs2A 114.6(2) . 1_455 ?
N11 C11 Cs6A 58.7(4) . 4_566 ?
Pt1 C11 Cs6A 119.9(2) . 4_566 ?
Cs2A C11 Cs6A 125.41(19) 1_455 4_566 ?
N11 C11 Cs2 71.9(4) . 1_455 ?
Pt1 C11 Cs2 109.4(2) . 1_455 ?
Cs2A C11 Cs2 11.24(3) 1_455 1_455 ?
Cs6A C11 Cs2 128.92(19) 4_566 1_455 ?
N11 C11 Cs6 64.9(4) . 4_566 ?
Pt1 C11 Cs6 113.7(2) . 4_566 ?
Cs2A C11 Cs6 131.63(19) 1_455 4_566 ?
```

```
Cs6A C11 Cs6 6.31(4) 4_566 4_566 ?
Cs2 C11 Cs6 135.21(19) 1_455 4_566 ?
N12 C12 Pt1 177.2(6) . . ?
N12 C12 Cs6 65.2(5) . 4_566 ?
Pt1 C12 Cs6 112.0(2) . 4_566 ?
N13 C13 Pt1 176.2(6) . . ?
N13 C13 Cs3A 63.2(4) . 1_655 ?
Pt1 C13 Cs3A 119.6(3) . 1_655 ?
N13 C13 Cs3 60.8(4) . 1_655 ?
Pt1 C13 Cs3 121.8(2) . 1_655 ?
Cs3A C13 Cs3 4.42(19) 1_655 1_655 ?
N13 C13 Cs6 59.6(4) . . ?
Pt1 C13 Cs6 116.9(2) . . ?
Cs3A C13 Cs6 120.5(3) 1_655 . ?
Cs3 C13 Cs6 117.1(2) 1_655 . ?
N13 C13 Cs1 112.7(5) . . ?
Pt1 C13 Cs1 68.69(18) . . ?
Cs3A C13 Cs1 118.1(3) 1_655 . ?
Cs3 C13 Cs1 122.23(19) 1_655 . ?
Cs6 C13 Cs1 97.88(14) . . ?
N13 C13 Cs1A 113.5(5) . . ?
Pt1 C13 Cs1A 68.2(2) . . ?
Cs3A C13 Cs1A 113.9(3) 1_655 . ?
Cs3 C13 Cs1A 118.1(3) 1_655 . ?
Cs6 C13 Cs1A 102.5(2) . . ?
Cs1 C13 Cs1A 4.90(15) . . ?
N13 C13 Cs6A 65.5(4) . . ?
Pt1 C13 Cs6A 111.0(2) . . ?
Cs3A C13 Cs6A 126.1(3) 1_655 . ?
Cs3 C13 Cs6A 122.5(2) 1_655 . ?
Cs6 C13 Cs6A 5.94(4) . . ?
Cs1 C13 Cs6A 95.98(14) . . ?
Cs1A C13 Cs6A 100.8(2) . . ?
N14 C14 Pt1 176.9(6) . . ?
N14 C14 Cs2 69.1(4) . 1_455 ?
Pt1 C14 Cs2 113.4(2) . 1_455 ?
N14 C14 Cs6A 59.0(4) . . ?
Pt1 C14 Cs6A 118.3(2) . . ?
Cs2 C14 Cs6A 127.48(18) 1_455 . ?
N14 C14 Cs1 111.8(4) . . ?
Pt1 C14 Cs1 69.54(17) . . ?
Cs2 C14 Cs1 106.06(15) 1_455 . ?
Cs6A C14 Cs1 100.00(14) . . ?
N14 C14 Cs2A 74.8(4) . 1_455 ?
Pt1 C14 Cs2A 107.9(2) . 1_455 ?
Cs2 C14 Cs2A 10.78(3) 1_455 1_455 ?
Cs6A C14 Cs2A 133.79(18) . 1_455 ?
Cs1 C14 Cs2A 95.54(14) . 1_455 ?
N14 C14 Cs6 64.5(4) . . ?
Pt1 C14 Cs6 112.8(2) . . ?
Cs2 C14 Cs6 133.19(17) 1_455 . ?
Cs6A C14 Cs6 5.73(6) . . ?
Cs1 C14 Cs6 96.74(13) . . ?
Cs2A C14 Cs6 139.25(17) 1_455 . ?
C11 N11 Cs6A 103.6(5) . 4_566 ?
C11 N11 Cs3A 119.5(6) . . ?
Cs6A N11 Cs3A 75.48(19) 4_566 . ?
```

```
C11 N11 Cs2A 94.7(5) . 1_455 ?
Cs6A N11 Cs2A 161.5(2) 4_566 1_455 ?
Cs3A N11 Cs2A 93.2(2) . 1_455 ?
C11 N11 Cs3 114.4(5) . . ?
Cs6A N11 Cs3 75.77(16) 4_566 . ?
Cs3A N11 Cs3 5.1(2) . . ?
Cs2A N11 Cs3 94.24(15) 1_455 . ?
C11 N11 Cs6 97.4(5) . 4_566 ?
Cs6A N11 Cs6 6.39(5) 4_566 4_566 ?
Cs3A N11 Cs6 79.70(19) . 4_566 ?
Cs2A N11 Cs6 167.8(2) 1_455 4_566 ?
Cs3 N11 Cs6 79.53(15) . 4_566 ?
C11 N11 Cs2 90.0(4) . 1_455 ?
Cs6A N11 Cs2 160.9(2) 4_566 1_455 ?
Cs3A N11 Cs2 86.21(18) . 1_455 ?
Cs2A N11 Cs2 11.68(4) 1_455 1_455 ?
Cs3 N11 Cs2 86.49(14) . 1_455 ?
Cs6 N11 Cs2 165.9(2) 4_566 1_455 ?
C12 N12 Cs2 122.1(5) . 4_566 ?
C12 N12 Cs4 140.5(5) . 4_666 ?
Cs2 N12 Cs4 94.31(16) 4_566 4_666 ?
C12 N12 Cs6 97.3(5) . 4_566 ?
Cs2 N12 Cs6 81.72(16) 4_566 4_566 ?
Cs4 N12 Cs6 103.08(19) 4_666 4_566 ?
C12 N12 Cs4A 138.4(5) . 4_666 ?
Cs2 N12 Cs4A 98.67(15) 4_566 4_666 ?
Cs4 N12 Cs4A 8.70(4) 4_666 4_666 ?
Cs6 N12 Cs4A 96.17(18) 4_566 4_666 ?
C12 N12 Cs2A 114.5(5) . 4_566 ?
Cs2 N12 Cs2A 7.83(3) 4_566 4_566 ?
Cs4 N12 Cs2A 100.93(16) 4_666 4_566 ?
Cs6 N12 Cs2A 84.38(15) 4_566 4_566 ?
Cs4A N12 Cs2A 105.78(15) 4_666 4_566 ?
C12 N12 Cs6A 93.2(5) . 4_566 ?
Cs2 N12 Cs6A 84.28(16) 4_566 4_566 ?
Cs4 N12 Cs6A 106.2(2) 4_666 4_566 ?
Cs6 N12 Cs6A 4.11(7) 4_566 4_566 ?
Cs4A N12 Cs6A 99.02(18) 4_666 4_566 ?
Cs2A N12 Cs6A 86.50(15) 4_566 4_566 ?
C13 N13 Cs3A 97.6(5) . 1_655 ?
C13 N13 Cs2 133.2(6) . . ?
Cs3A N13 Cs2 94.0(2) 1_655 . ?
C13 N13 Cs3 101.0(4) . 1_655 ?
Cs3A N13 Cs3 5.4(2) 1_655 1_655 ?
Cs2 N13 Cs3 94.50(15) . 1_655 ?
C13 N13 Cs6 102.8(5) . . ?
Cs3A N13 Cs6 153.5(4) 1_655 . ?
Cs2 N13 Cs6 84.29(15) . . ?
Cs3 N13 Cs6 148.2(3) 1_655 . ?
C13 N13 Cs2A 122.6(6) . . ?
Cs3A N13 Cs2A 92.2(2) 1_655 . ?
Cs2 N13 Cs2A 11.35(4) . . ?
Cs3 N13 Cs2A 93.75(16) 1_655 . ?
Cs6 N13 Cs2A 90.89(15) . . ?
C13 N13 Cs6A 97.2(4) . . ?
Cs3A N13 Cs6A 157.2(4) 1_655 . ?
Cs2 N13 Cs6A 88.43(16) . . ?
```

```
Cs3 N13 Cs6A 151.8(3) 1_655 . ?
Cs6 N13 Cs6A 5.67(5) . . ?
Cs2A N13 Cs6A 94.34(16) . . ?
C13 N13 Cs5 117.1(5) . . ?
Cs3A N13 Cs5 75.3(3) 1_655 . ?
Cs2 N13 Cs5 109.76(19) . . ?
Cs3 N13 Cs5 70.03(15) 1_655 . ?
Cs6 N13 Cs5 80.46(17) . . ?
Cs2A N13 Cs5 120.14(18) . . ?
Cs6A N13 Cs5 82.62(17) . . ?
C14 N14 Cs3A 140.0(6) . 4_565 ?
C14 N14 Cs3 134.3(5) . 4_565 ?
Cs3A N14 Cs3 5.8(2) 4_565 4_565 ?
C14 N14 Cs6A 103.2(5) . . ?
Cs3A N14 Cs6A 77.7(2) 4_565 . ?
Cs3 N14 Cs6A 79.01(14) 4_565 . ?
C14 N14 Cs2 92.1(4) . 1_455 ?
Cs3A N14 Cs2 95.94(19) 4_565 1_455 ?
Cs3 N14 Cs2 96.30(15) 4_565 1_455 ?
Cs6A N14 Cs2 162.7(2) . 1_455 ?
C14 N14 Cs6 98.1(4) . . ?
Cs3A N14 Cs6 80.47(18) 4_565 . ?
Cs3 N14 Cs6 81.31(13) 4_565 . ?
Cs6A N14 Cs6 5.26(8) . . ?
Cs2 N14 Cs6 167.8(2) 1_455 . ?
C14 N14 Cs4 121.6(4) . . ?
Cs3A N14 Cs4 98.1(3) 4_565 . ?
Cs3 N14 Cs4 103.85(18) 4_565 . ?
Cs6A N14 Cs4 79.48(17) . . ?
Cs2 N14 Cs4 85.56(12) 1_455 . ?
Cs6 N14 Cs4 83.41(16) . . ?
C14 N14 Cs2A 87.4(5) . 1_455 ?
Cs3A N14 Cs2A 93.4(2) 4_565 1_455 ?
Cs3 N14 Cs2A 92.72(15) 4_565 1_455 ?
Cs6A N14 Cs2A 169.35(19) . 1_455 ?
Cs2 N14 Cs2A 10.69(4) 1_455 1_455 ?
Cs6 N14 Cs2A 173.72(17) . 1_455 ?
Cs4 N14 Cs2A 96.20(13) . 1_455 ?
C21 Pt2 C24 90.7(2) . . ?
C21 Pt2 C22 88.6(2) . . ?
C24 Pt2 C22 178.76(19) . . ?
C21 Pt2 C23 179.9(2) . . ?
C24 Pt2 C23 89.20(19) . . ?
C22 Pt2 C23 91.46(19) . . ?
C21 Pt2 Pt3 87.95(14) . 2_655 ?
C24 Pt2 Pt3 88.09(14) . 2_655 ?
C22 Pt2 Pt3 90.84(13) . 2_655 ?
C23 Pt2 Pt3 92.17(14) . 2_655 ?
C21 Pt2 Pt1 91.48(14) . . ?
C24 Pt2 Pt1 93.00(14) . . ?
C22 Pt2 Pt1 88.07(13) . . ?
C23 Pt2 Pt1 88.40(14) . . ?
Pt3 Pt2 Pt1 178.778(7) 2_655 . ?
N21 C21 Pt2 178.5(5) . . ?
N21 C21 Cs5 68.6(4) . . ?
Pt2 C21 Cs5 111.76(19) . . ?
N21 C21 Cs2A 64.4(3) . 4_566 ?
```

```
Pt2 C21 Cs2A 115.2(2) . 4_566 ?
Cs5 C21 Cs2A 132.91(15) . 4_566 ?
N21 C21 Cs3 44.2(3) . 1_655 ?
Pt2 C21 Cs3 137.2(2) . 1_655 ?
Cs5 C21 Cs3 65.07(10) . 1_655 ?
Cs2A C21 Cs3 82.57(11) 4_566 1_655 ?
N21 C21 Cs2 67.5(4) . 4_566 ?
Pt2 C21 Cs2 112.35(19) . 4_566 ?
Cs5 C21 Cs2 135.30(14) . 4_566 ?
Cs2A C21 Cs2 10.48(3) 4_566 4_566 ?
Cs3 C21 Cs2 77.86(10) 1_655 4_566 ?
N21 C21 Cs3A 48.0(4) . 1_655 ?
Pt2 C21 Cs3A 133.4(3) . 1_655 ?
Cs5 C21 Cs3A 68.4(2) . 1_655 ?
Cs2A C21 Cs3A 81.87(14) 4_566 1_655 ?
Cs3 C21 Cs3A 4.69(17) 1_655 1_655 ?
Cs2 C21 Cs3A 76.43(15) 4_566 1_655 ?
N22 C22 Pt2 178.5(5) . . ?
N22 C22 Cs3 70.8(3) . . ?
Pt2 C22 Cs3 110.23(17) . . ?
N22 C22 Cs2A 67.3(3) . 4_566 ?
Pt2 C22 Cs2A 111.61(18) . 4_566 ?
Cs3 C22 Cs2A 138.15(15) . 4_566 ?
N22 C22 Cs3A 69.9(3) . . ?
Pt2 C22 Cs3A 111.2(2) . . ?
Cs3 C22 Cs3A 3.83(15) . . ?
Cs2A C22 Cs3A 137.08(18) 4_566 . ?
N22 C22 Cs2 64.0(3) . 4_566 ?
Pt2 C22 Cs2 115.11(18) . 4_566 ?
Cs3 C22 Cs2 133.57(15) . 4_566 ?
Cs2A C22 Cs2 11.02(3) 4_566 4_566 ?
Cs3A C22 Cs2 131.64(19) . 4_566 ?
N23 C23 Pt2 179.1(5) . . ?
N23 C23 Cs3 70.1(3) . . ?
Pt2 C23 Cs3 110.70(18) . . ?
N23 C23 Cs4 65.4(3) . . ?
Pt2 C23 Cs4 113.76(18) . . ?
Cs3 C23 Cs4 135.48(15) . . ?
N23 C23 Cs3A 68.7(3) . . ?
Pt2 C23 Cs3A 112.1(2) . . ?
Cs3 C23 Cs3A 4.00(15) . . ?
Cs4 C23 Cs3A 134.06(19) . . ?
N23 C23 Cs4A 64.4(3) . . ?
Pt2 C23 Cs4A 114.73(18) . . ?
Cs3 C23 Cs4A 133.11(15) . . ?
Cs4 C23 Cs4A 8.86(3) . . ?
Cs3A C23 Cs4A 132.50(17) . . ?
N23 C23 Cs5 44.6(3) . 1_455 ?
Pt2 C23 Cs5 135.31(19) . 1_455 ?
Cs3 C23 Cs5 64.78(9) . 1_455 ?
Cs4 C23 Cs5 81.93(10) . 1_455 ?
Cs3A C23 Cs5 66.62(15) . 1_455 ?
Cs4A C23 Cs5 75.00(10) . 1_455 ?
N24 C24 Pt2 178.0(4) . . ?
N24 C24 Cs5 69.5(3) . . ?
Pt2 C24 Cs5 110.59(18) . . ?
N24 C24 Cs4 67.9(3) . . ?
```

```
Pt2 C24 Cs4 111.96(18) . . ?
Cs5 C24 Cs4 137.39(15) . . ?
N24 C24 Cs6A 45.7(3) . . ?
Pt2 C24 Cs6A 136.3(2) . . ?
Cs5 C24 Cs6A 80.41(11) . . ?
Cs4 C24 Cs6A 70.70(10) . . ?
N24 C24 Cs6 46.0(3) . . ?
Pt2 C24 Cs6 136.1(2) . . ?
Cs5 C24 Cs6 74.64(10) . . ?
Cs4 C24 Cs6 76.63(10) . . ?
Cs6A C24 Cs6 6.09(4) . . ?
N24 C24 Cs4A 67.6(3) . . ?
Pt2 C24 Cs4A 111.92(17) . . ?
Cs5 C24 Cs4A 136.00(15) . . ?
Cs4 C24 Cs4A 8.57(3) . . ?
Cs6A C24 Cs4A 76.89(11) . . ?
Cs6 C24 Cs4A 82.63(11) . . ?
C21 N21 Cs3 120.9(4) . 1_655 ?
C21 N21 Cs3A 116.6(5) . 1_655 ?
Cs3 N21 Cs3A 5.5(2) 1_655 1_655 ?
C21 N21 Cs2A 97.2(4) . 4_566 ?
Cs3 N21 Cs2A 100.34(16) 1_655 4_566 ?
Cs3A N21 Cs2A 98.0(2) 1_655 4_566 ?
C21 N21 Cs5 92.5(4) . . ?
Cs3 N21 Cs5 76.53(12) 1_655 . ?
Cs3A N21 Cs5 79.7(2) 1_655 . ?
Cs2A N21 Cs5 170.07(17) 4_566 . ?
C21 N21 Cs5A 118.9(4) . 3_766 ?
Cs3 N21 Cs5A 114.98(17) 1_655 3_766 ?
Cs3A N21 Cs5A 120.3(3) 1_655 3_766 ?
Cs2A N21 Cs5A 95.37(13) 4_566 3_766 ?
Cs5 N21 Cs5A 77.78(12) . 3_766 ?
C21 N21 Cs2 95.1(4) . 4_566 ?
Cs3 N21 Cs2 92.21(14) 1_655 4_566 ?
Cs3A N21 Cs2 89.3(2) 1_655 4_566 ?
Cs2A N21 Cs2 11.09(4) 4_566 4_566 ?
Cs5 N21 Cs2 168.56(16) . 4_566 ?
Cs5A N21 Cs2 105.77(13) 3_766 4_566 ?
C21 N21 Cs5A 95.8(4) . . ?
Cs3 N21 Cs5A 80.39(12) 1_655 . ?
Cs3A N21 Cs5A 84.0(2) 1_655 . ?
Cs2A N21 Cs5A 164.26(18) 4_566 . ?
Cs5 N21 Cs5A 7.30(3) . . ?
Cs5A N21 Cs5A 70.48(11) 3_766 . ?
Cs2 N21 Cs5A 168.86(15) 4_566 . ?
C22 N22 Cs6 123.7(4) . 4_566 ?
C22 N22 Cs6A 123.9(4) . 4_566 ?
Cs6 N22 Cs6A 7.35(5) 4_566 4_566 ?
C22 N22 Cs3 90.3(3) . . ?
Cs6 N22 Cs3 83.32(14) 4_566 . ?
Cs6A N22 Cs3 76.04(14) 4_566 . ?
C22 N22 Cs1 116.2(4) . 4_566 ?
Cs6 N22 Cs1 119.92(14) 4_566 4_566 ?
Cs6A N22 Cs1 118.59(14) 4_566 4_566 ?
Cs3 N22 Cs1 93.09(13) . 4_566 ?
C22 N22 Cs2 98.4(3) . 4_566 ?
Cs6 N22 Cs2 82.51(11) 4_566 4_566 ?
```

```
Cs6A N22 Cs2 89.77(13) 4_566 4_566 ?
Cs3 N22 Cs2 165.80(17) . 4_566 ?
Cs1 N22 Cs2 93.11(12) 4_566 4_566 ?
C22 N22 Cs2A 94.7(3) . 4_566 ?
Cs6 N22 Cs2A 94.11(13) 4_566 4_566 ?
Cs6A N22 Cs2A 101.29(14) 4_566 4_566 ?
Cs3 N22 Cs2A 175.03(15) . 4_566 ?
Cs1 N22 Cs2A 84.48(12) 4_566 4_566 ?
Cs2 N22 Cs2A 12.06(3) 4_566 4_566 ?
C22 N22 Cs3A 92.3(4) . . ?
Cs6 N22 Cs3A 78.9(2) 4_566 . ?
Cs6A N22 Cs3A 71.7(2) 4_566 . ?
Cs3 N22 Cs3A 4.42(17) . . ?
Cs1 N22 Cs3A 95.7(2) 4_566 . ?
Cs2 N22 Cs3A 161.4(3) 4_566 . ?
Cs2A N22 Cs3A 172.1(2) 4_566 . ?
C22 N22 Cs1A 117.0(4) . 4_566 ?
Cs6 N22 Cs1A 119.29(16) 4_566 4_566 ?
Cs6A N22 Cs1A 118.46(17) 4_566 4_566 ?
Cs3 N22 Cs1A 96.41(19) . 4_566 ?
Cs1 N22 Cs1A 3.45(13) 4_566 4_566 ?
Cs2 N22 Cs1A 89.67(19) 4_566 4_566 ?
Cs2A N22 Cs1A 81.10(19) 4_566 4_566 ?
Cs3A N22 Cs1A 99.0(2) . 4_566 ?
C23 N23 Cs5 120.7(4) . 1_455 ?
C23 N23 Cs4 96.3(3) . . ?
Cs5 N23 Cs4 98.87(14) 1_455 . ?
C23 N23 Cs3 90.9(3) . . ?
Cs5 N23 Cs3 75.65(11) 1_455 . ?
Cs4 N23 Cs3 172.57(17) . . ?
C23 N23 Cs2 119.4(4) . 1_455 ?
Cs5 N23 Cs2 117.92(14) 1_455 1_455 ?
Cs4 N23 Cs2 88.81(11) . 1_455 ?
Cs3 N23 Cs2 89.41(14) . 1_455 ?
C23 N23 Cs5A 114.6(4) . 1_455 ?
Cs5 N23 Cs5A 8.59(3) 1_455 1_455 ?
Cs4 N23 Cs5A 94.05(13) . 1_455 ?
Cs3 N23 Cs5A 81.11(11) . 1_455 ?
Cs2 N23 Cs5A 125.24(15) 1_455 1_455 ?
C23 N23 Cs4A 98.2(4) . . ?
Cs5 N23 Cs4A 89.62(13) 1_455 . ?
Cs4 N23 Cs4A 9.85(4) . . ?
Cs3 N23 Cs4A 165.17(17) . . ?
Cs2 N23 Cs4A 96.17(12) 1_455 . ?
Cs5A N23 Cs4A 84.45(12) 1_455 . ?
C23 N23 Cs3A 93.4(4) . . ?
Cs5 N23 Cs3A 77.79(18) 1_455 . ?
Cs4 N23 Cs3A 170.2(2) . . ?
Cs3 N23 Cs3A 4.69(17) . . ?
Cs2 N23 Cs3A 84.7(3) 1_455 . ?
Cs5A N23 Cs3A 83.72(19) 1_455 . ?
Cs4A N23 Cs3A 166.08(19) . . ?
C24 N24 Cs6A 118.7(4) . . ?
C24 N24 Cs6 118.8(4) . . ?
Cs6A N24 Cs6 7.44(5) . . ?
C24 N24 Cs1A 124.1(4) . 2_655 ?
Cs6A N24 Cs1A 116.2(2) . 2_655 ?
```

```
Cs6 N24 Cs1A 117.0(2) . 2_655 ?
C24 N24 Cs1 120.5(4) . 2_655 ?
Cs6A N24 Cs1 120.43(17) . 2_655 ?
Cs6 N24 Cs1 120.71(15) . 2_655 ?
Cs1A N24 Cs1 5.49(17) 2_655 2_655 ?
C24 N24 Cs5 91.6(3) . . ?
Cs6A N24 Cs5 95.09(14) . . ?
Cs6 N24 Cs5 87.66(12) . . ?
Cs1A N24 Cs5 93.4(2) 2_655 . ?
Cs1 N24 Cs5 89.41(13) 2_655 . ?
C24 N24 Cs4 93.8(3) . . ?
Cs6A N24 Cs4 83.02(13) . . ?
Cs6 N24 Cs4 90.45(12) . . ?
Cs1A N24 Cs4 83.0(2) 2_655 . ?
Cs1 N24 Cs4 87.21(12) 2_655 . ?
Cs5 N24 Cs4 174.60(16) . . ?
C24 N24 Cs5A 95.8(3) . . ?
Cs6A N24 Cs5A 98.61(14) . . ?
Cs6 N24 Cs5A 91.26(12) . . ?
Cs1A N24 Cs5A 85.7(2) 2_655 . ?
Cs1 N24 Cs5A 81.72(12) 2_655 . ?
Cs5 N24 Cs5A 7.71(2) . . ?
Cs4 N24 Cs5A 168.01(16) . . ?
C24 N24 Cs4A 95.1(3) . . ?
Cs6A N24 Cs4A 90.49(14) . . ?
Cs6 N24 Cs4A 97.84(13) . . ?
Cs1A N24 Cs4A 74.6(2) 2_655 . ?
Cs1 N24 Cs4A 78.58(12) 2_655 . ?
Cs5 N24 Cs4A 167.97(16) . . ?
Cs4 N24 Cs4A 9.32(3) . . ?
Cs5A N24 Cs4A 160.26(16) . . ?
C32 Pt3 C32 180.0(4) . 3_655 ?
C32 Pt3 C31 90.2(2) . . ?
C32 Pt3 C31 89.8(2) 3_655 . ?
C32 Pt3 C31 89.8(2) . 3_655 ?
C32 Pt3 C31 90.2(2) 3_655 3_655 ?
C31 Pt3 C31 180.0(3) . 3_655 ?
C32 Pt3 Pt2 90.03(15) . 4_565 ?
C32 Pt3 Pt2 89.97(15) 3_655 4_565 ?
C31 Pt3 Pt2 87.03(14) . 4_565 ?
C31 Pt3 Pt2 92.97(14) 3_655 4_565 ?
C32 Pt3 Pt2 89.97(15) . 2_645 ?
C32 Pt3 Pt2 90.03(15) 3_655 2_645 ?
C31 Pt3 Pt2 92.97(14) . 2_645 ?
C31 Pt3 Pt2 87.03(14) 3_655 2_645 ?
Pt2 Pt3 Pt2 180.000(7) 4_565 2_645 ?
N31 C31 Pt3 179.2(5) . . ?
N31 C31 Cs5A 64.0(3) . 4_465 ?
Pt3 C31 Cs5A 115.4(2) . 4_465 ?
N31 C31 Cs1 68.1(3) . . ?
Pt3 C31 Cs1 112.48(19) . . ?
Cs5A C31 Cs1 132.06(15) 4_465 . ?
N31 C31 Cs5 59.2(3) . 4_465 ?
Pt3 C31 Cs5 120.13(19) . 4_465 ?
Cs5A C31 Cs5 8.15(2) 4_465 4_465 ?
Cs1 C31 Cs5 127.11(14) . 4_465 ?
N31 C31 Cs1A 70.5(4) . . ?
```

```
Pt3 C31 Cs1A 110.2(2) . . ?
Cs5A C31 Cs1A 134.18(19) 4_465 . ?
Cs1 C31 Cs1A 3.55(12) . . ?
Cs5 C31 Cs1A 129.63(19) 4_465 . ?
N31 C31 Cs5A 43.2(3) . 2_645 ?
Pt3 C31 Cs5A 137.3(2) . 2_645 ?
Cs5A C31 Cs5A 68.01(9) 4_465 2_645 ?
Cs1 C31 Cs5A 76.01(9) . 2_645 ?
Cs5 C31 Cs5A 69.61(9) 4_465 2_645 ?
Cs1A C31 Cs5A 75.79(14) . 2_645 ?
C31 N31 Cs5A 122.3(4) . 2_645 ?
C31 N31 Cs5A 96.9(4) . 4_465 ?
Cs5A N31 Cs5A 81.99(12) 2_645 4_465 ?
C31 N31 Cs5 103.0(4) . 4_465 ?
Cs5A N31 Cs5 85.08(12) 2_645 4_465 ?
Cs5A N31 Cs5 9.56(2) 4_465 4_465 ?
C31 N31 Cs1 92.8(4) . . ?
Cs5A N31 Cs1 90.80(12) 2_645 . ?
Cs5A N31 Cs1 170.02(16) 4_465 . ?
Cs5 N31 Cs1 163.46(17) 4_465 . ?
C31 N31 Cs5 113.5(4) . 2_645 ?
Cs5A N31 Cs5 8.81(3) 2_645 2_645 ?
Cs5A N31 Cs5 82.92(12) 4_465 2_645 ?
Cs5 N31 Cs5 87.34(12) 4_465 2_645 ?
Cs1 N31 Cs5 91.02(12) . 2_645 ?
C31 N31 Cs3 119.5(4) . 4_565 ?
Cs5A N31 Cs3 117.63(14) 2_645 4_565 ?
Cs5A N31 Cs3 82.91(11) 4_465 4_565 ?
Cs5 N31 Cs3 73.53(10) 4_465 4_565 ?
Cs1 N31 Cs3 94.44(13) . 4_565 ?
Cs5 N31 Cs3 126.37(14) 2_645 4_565 ?
C31 N31 Cs1A 91.6(4) . . ?
Cs5A N31 Cs1A 88.99(17) 2_645 . ?
Cs5A N31 Cs1A 169.94(19) 4_465 . ?
Cs5 N31 Cs1A 165.20(19) 4_465 . ?
Cs1 N31 Cs1A 3.06(12) . . ?
Cs5 N31 Cs1A 88.85(17) 2_645 . ?
Cs3 N31 Cs1A 97.47(19) 4_565 . ?
C31 N31 Cs3A 120.5(4) . 4_565 ?
Cs5A N31 Cs3A 116.62(17) 2_645 4_565 ?
Cs5A N31 Cs3A 82.79(14) 4_465 4_565 ?
Cs5 N31 Cs3A 73.38(14) 4_465 4_565 ?
Cs1 N31 Cs3A 94.39(16) . 4_565 ?
Cs5 N31 Cs3A 125.36(17) 2_645 4_565 ?
Cs3 N31 Cs3A 1.02(11) 4_565 4_565 ?
Cs1A N31 Cs3A 97.4(2) . 4_565 ?
N32 C32 Pt3 179.9(6) . . ?
N32 C32 Cs1 69.9(4) . . ?
Pt3 C32 Cs1 110.0(2) . . ?
N32 C32 Cs1A 65.9(4) . . ?
Pt3 C32 Cs1A 114.1(3) . . ?
Cs1 C32 Cs1A 5.08(15) . . ?
N32 C32 Cs5A 71.6(4) . 2_745 ?
Pt3 C32 Cs5A 108.44(19) . 2_745 ?
Cs1 C32 Cs5A 141.49(18) . 2_745 ?
Cs1A C32 Cs5A 137.1(3) . 2_745 ?
N32 C32 Cs4A 39.4(3) . 2_645 ?
```

```
Pt3 C32 Cs4A 140.6(2) . 2_645 ?
Cs1 C32 Cs4A 73.00(12) . 2_645 ?
Cs1A C32 Cs4A 67.9(2) . 2_645 ?
Cs5A C32 Cs4A 75.91(11) 2_745 2_645 ?
C32 N32 Cs4A 126.5(4) . 2_645 ?
C32 N32 Cs1A 95.6(4) . . ?
Cs4A N32 Cs1A 81.9(3) 2_645 . ?
C32 N32 Cs1 91.1(4) . . ?
Cs4A N32 Cs1 87.22(16) 2_645 . ?
Cs1A N32 Cs1 5.56(17) . . ?
C32 N32 Cs2A 119.7(4) . . ?
Cs4A N32 Cs2A 113.50(17) 2_645 . ?
Cs1A N32 Cs2A 87.16(18) . . ?
Cs1 N32 Cs2A 86.54(14) . . ?
C32 N32 Cs4 118.7(4) . 2_645 ?
Cs4A N32 Cs4 7.83(5) 2_645 2_645 ?
Cs1A N32 Cs4 81.7(2) . 2_645 ?
Cs1 N32 Cs4 86.71(14) . 2_645 ?
Cs2A N32 Cs4 121.22(16) . 2_645 ?
C32 N32 Cs5A 90.0(4) . 2_745 ?
Cs4A N32 Cs5A 90.00(15) 2_645 2_745 ?
Cs1A N32 Cs5A 171.9(3) . 2_745 ?
Cs1 N32 Cs5A 177.1(2) . 2_745 ?
Cs2A N32 Cs5A 95.20(14) . 2_745 ?
Cs4 N32 Cs5A 90.45(13) 2_645 2_745 ?
C41 Pt4 C41 180.000(1) 3_656 . ?
C41 Pt4 C42 88.2(4) 3_656 . ?
C41 Pt4 C42 91.8(4) . . ?
C41 Pt4 C42 91.8(4) 3_656 3_656 ?
C41 Pt4 C42 88.2(4) . 3_656 ?
C42 Pt4 C42 180.000(1) . 3_656 ?
C41 Pt4 Cs6 63.0(3) 3_656 4_566 ?
C41 Pt4 Cs6 117.0(3) . 4_566 ?
C42 Pt4 Cs6 105.8(3) . 4_566 ?
C42 Pt4 Cs6 74.2(3) 3_656 4_566 ?
C41 Pt4 Cs6 117.0(3) 3_656 2_645 ?
C41 Pt4 Cs6 63.0(3) . 2_645 ?
C42 Pt4 Cs6 74.2(3) . 2_645 ?
C42 Pt4 Cs6 105.8(3) 3_656 2_645 ?
Cs6 Pt4 Cs6 180.0 4_566 2_645 ?
C41 Pt4 Cs6A 67.4(3) 3_656 4_566 ?
C41 Pt4 Cs6A 112.6(3) . 4_566 ?
C42 Pt4 Cs6A 110.7(3) . 4_566 ?
C42 Pt4 Cs6A 69.3(3) 3_656 4_566 ?
Cs6 Pt4 Cs6A 6.09(4) 4_566 4_566 ?
Cs6 Pt4 Cs6A 173.91(4) 2_645 4_566 ?
C41 Pt4 Cs6A 112.6(3) 3_656 2_645 ?
C41 Pt4 Cs6A 67.4(3) . 2_645 ?
C42 Pt4 Cs6A 69.3(3) . 2_645 ?
C42 Pt4 Cs6A 110.7(3) 3_656 2_645 ?
Cs6 Pt4 Cs6A 173.91(4) 4_566 2_645 ?
Cs6 Pt4 Cs6A 6.09(4) 2_645 2_645 ?
Cs6A Pt4 Cs6A 180.0 4_566 2_645 ?
N41 C41 Pt4 179.0(14) . . ?
N41 C41 Cs4A 61.3(9) . 2_545 ?
Pt4 C41 Cs4A 119.7(5) . 2_545 ?
N41 C41 Cs6 93.4(8) . 2_645 ?
```

```
Pt4 C41 Cs6 86.8(3) . 2_645 ?
Cs4A C41 Cs6 98.8(3) 2_545 2_645 ?
N41 C41 Cs6A 97.3(8) . 2_645 ?
Pt4 C41 Cs6A 82.8(3) . 2_645 ?
Cs4A C41 Cs6A 104.8(3) 2_545 2_645 ?
Cs6 C41 Cs6A 6.11(6) 2_645 2_645 ?
N41 C41 Cs4 64.2(9) . 2_545 ?
Pt4 C41 Cs4 116.8(5) . 2_545 ?
Cs4A C41 Cs4 7.23(5) 2_545 2_545 ?
Cs6 C41 Cs4 92.2(3) 2_645 2_545 ?
Cs6A C41 Cs4 98.1(3) 2_645 2_545 ?
C41 N41 Cs5A 155.2(8) . 2_645 ?
C41 N41 Cs4A 99.4(10) . 2_545 ?
Cs5A N41 Cs4A 100.2(3) 2_645 2_545 ?
C41 N41 Cs5 148.2(8) . 2_645 ?
Cs5A N41 Cs5 9.92(4) 2_645 2_645 ?
Cs4A N41 Cs5 100.1(4) 2_545 2_645 ?
C41 N41 Cs4 98.5(10) . 2_545 ?
Cs5A N41 Cs4 99.0(3) 2_645 2_545 ?
Cs4A N41 Cs4 7.39(7) 2_545 2_545 ?
Cs5 N41 Cs4 97.7(3) 2_645 2_545 ?
C41 N41 Cs6 68.7(8) . 2_645 ?
Cs5A N41 Cs6 92.7(3) 2_645 2_645 ?
Cs4A N41 Cs6 101.0(5) 2_545 2_645 ?
Cs5 N41 Cs6 83.0(3) 2_645 2_645 ?
Cs4 N41 Cs6 93.8(4) 2_545 2_645 ?
N42 C42 Pt4 179.3(9) . . ?
N42 C42 Cs1A 58.3(7) . . ?
Pt4 C42 Cs1A 121.2(4) . . ?
N42 C42 Cs6A 99.3(8) . 2_645 ?
Pt4 C42 Cs6A 80.1(4) . 2_645 ?
Cs1A C42 Cs6A 97.1(2) . 2_645 ?
N42 C42 Cs4A 74.9(6) . 4_666 ?
Pt4 C42 Cs4A 105.8(3) . 4_666 ?
Cs1A C42 Cs4A 121.7(4) . 4_666 ?
Cs6A C42 Cs4A 124.9(3) 2_645 4_666 ?
N42 C42 Cs1 60.6(7) . . ?
Pt4 C42 Cs1 118.9(3) . . ?
Cs1A C42 Cs1 2.32(14) . . ?
Cs6A C42 Cs1 96.50(17) 2_645 . ?
Cs4A C42 Cs1 123.6(4) 4_666 . ?
N42 C42 Cs6 103.8(8) . 2_645 ?
Pt4 C42 Cs6 75.6(3) . 2_645 ?
Cs1A C42 Cs6 96.2(2) . 2_645 ?
Cs6A C42 Cs6 5.85(4) 2_645 2_645 ?
Cs4A C42 Cs6 129.3(3) 4_666 2_645 ?
Cs1 C42 Cs6 95.44(16) . 2_645 ?
C42 N42 Cs1A 102.9(7) . . ?
C42 N42 Cs4A 145.4(10) . 2_645 ?
Cs1A N42 Cs4A 82.5(3) . 2_645 ?
C42 N42 Cs4 135.3(10) . 2_645 ?
Cs1A N42 Cs4 87.6(2) . 2_645 ?
Cs4A N42 Cs4 10.43(5) 2_645 2_645 ?
C42 N42 Cs1 102.0(7) . . ?
Cs1A N42 Cs1 0.94(15) . . ?
Cs4A N42 Cs1 83.0(2) 2_645 . ?
Cs4 N42 Cs1 88.0(2) 2_645 . ?
```

```
C42 N42 Cs4A 87.0(6) . 4_666 ?
Cs1A N42 Cs4A 142.8(5) . 4_666 ?
Cs4A N42 Cs4A 109.6(2) 2_645 4_666 ?
Cs4 N42 Cs4A 110.7(2) 2_645 4_666 ?
Cs1 N42 Cs4A 143.2(4) . 4_666 ?
C42 N42 Cs4 91.9(6) . 4_666 ?
Cs1A N42 Cs4 133.8(5) . 4_666 ?
Cs4A N42 Cs4 109.1(3) 2_645 4_666 ?
Cs4 N42 Cs4 111.9(2) 2_645 4_666 ?
Cs1 N42 Cs4 134.3(4) . 4_666 ?
Cs4A N42 Cs4 9.22(4) 4_666 4_666 ?
Cs2A O1 Cs5A 122.1(3) 1_455 2_645 ?
Cs2A O1 Cs1 143.3(3) 1_455 . ?
Cs5A O1 Cs1 94.5(2) 2_645 . ?
Cs2A O1 Cs2 10.38(6) 1_455 1_455 ?
Cs5A O1 Cs2 130.1(3) 2_645 1_455 ?
Cs1 O1 Cs2 134.5(3) . 1_455 ?
Cs2A O1 Cs1A 143.2(3) 1_455 . ?
Cs5A O1 Cs1A 94.5(2) 2_645 . ?
Cs1 O1 Cs1A 4.96(15) . . ?
Cs2 O1 Cs1A 135.1(3) 1_455 . ?
Cs2A O1 Cs5 126.5(3) 1_455 2_645 ?
Cs5A O1 Cs5 5.45(4) 2_645 2_645 ?
Cs1 O1 Cs5 90.17(19) . 2_645 ?
Cs2 O1 Cs5 134.9(3) 1_455 2_645 ?
Cs1A O1 Cs5 89.9(2) . 2_645 ?
O2A O2 Cs2A 127(2) 1_655 . ?
O2A O2 Cs4A 99(2) 1_655 2_645 ?
Cs2A O2 Cs4A 131.5(6) . 2_645 ?
O2A O2 Cs2 119(2) 1_655 . ?
Cs2A O2 Cs2 8.93(8) . . ?
Cs4A O2 Cs2 140.3(5) 2_645 . ?
O2A O2 Cs1A 71.9(19) 1_655 . ?
Cs2A O2 Cs1A 98.3(4) . . ?
Cs4A O2 Cs1A 80.6(3) 2_645 . ?
Cs2 O2 Cs1A 98.0(4) . . ?
O2A O2 Cs1 75.1(19) 1_655 . ?
Cs2A O2 Cs1 93.9(4) . . ?
Cs4A O2 Cs1 83.1(3) 2_645 . ?
Cs2 O2 Cs1 93.6(3) . . ?
Cs1A O2 Cs1 4.51(16) . . ?
O2A O2 Cs4 96(2) 1_655 2_645 ?
Cs2A O2 Cs4 133.8(5) . 2_645 ?
Cs4A O2 Cs4 3.37(6) 2_645 2_645 ?
Cs2 O2 Cs4 142.5(5) . 2_645 ?
Cs1A O2 Cs4 78.1(3) . 2_645 ?
Cs1 O2 Cs4 80.7(3) . 2_645 ?
O2 O2A O3A 148(6) 1_455 . ?
O2 O2A Cs1A 94(2) 1_455 1_455 ?
O3A O2A Cs1A 117(5) . 1_455 ?
O2 O2A Cs2A 41(2) 1_455 1_455 ?
O3A O2A Cs2A 138(5) . 1_455 ?
Cs1A O2A Cs2A 90.9(7) 1_455 1_455 ?
O2 O2A Cs4A 68(2) 1_455 2_545 ?
O3A O2A Cs4A 108(5) . 2_545 ?
Cs1A O2A Cs4A 79.7(6) 1_455 2_545 ?
Cs2A O2A Cs4A 107.3(9) 1_455 2_545 ?
```

```
O2 O2A Cs1 92(2) 1_455 1_455 ?
O3A O2A Cs1 120(5) . 1_455 ?
Cs1A O2A Cs1 4.14(17) 1_455 1_455 ?
Cs2A O2A Cs1 86.8(7) 1_455 1_455 ?
Cs4A O2A Cs1 81.8(5) 2_545 1_455 ?
O2 O2A Cs2 50(2) 1_455 1_455 ?
O3A O2A Cs2 130(5) . 1_455 ?
Cs1A O2A Cs2 92.0(7) 1_455 1_455 ?
Cs2A O2A Cs2 9.18(9) 1_455 1_455 ?
Cs4A O2A Cs2 116.5(9) 2_545 1_455 ?
Cs1 O2A Cs2 87.9(6) 1_455 1_455 ?
O3A O3 Cs3A 115(5) . . ?
O3A O3 Cs4 117(6) . 4_566 ?
Cs3A O3 Cs4 119.1(9) . 4_566 ?
O3A O3 Cs3 116(5) . . ?
Cs3A O3 Cs3 1.79(16) . . ?
Cs4 O3 Cs3 118.7(8) 4_566 . ?
O3A O3 Cs4A 109(6) . 4_566 ?
Cs3A O3 Cs4A 126.7(8) . 4_566 ?
Cs4 O3 Cs4A 7.93(6) 4_566 4_566 ?
Cs3 O3 Cs4A 126.4(8) . 4_566 ?
O3A O3 Cs6A 137(6) . 4_566 ?
Cs3A O3 Cs6A 77.4(5) . 4_566 ?
Cs4 O3 Cs6A 85.8(6) 4_566 4_566 ?
Cs3 O3 Cs6A 75.6(4) . 4_566 ?
Cs4A O3 Cs6A 90.0(5) 4_566 4_566 ?
O3 O3A O2A 152(9) . . ?
O3 O3A Cs3A 51(4) . . ?
O2A O3A Cs3A 108(5) . . ?
O3 O3A Cs4 49(6) . 4_566 ?
O2A O3A Cs4 157(6) . 4_566 ?
Cs3A O3A Cs4 95(4) . 4_566 ?
O3 O3A Cs3 51(4) . . ?
O2A O3A Cs3 108(5) . . ?
Cs3A O3A Cs3 1.11(18) . . ?
Cs4 O3A Cs3 95(4) 4_566 . ?
O3 O3A Cs4A 57(6) . 4_566 ?
O2A O3A Cs4A 149(6) . 4_566 ?
Cs3A O3A Cs4A 103(4) . 4_566 ?
Cs4 O3A Cs4A 8.2(2) 4_566 4_566 ?
Cs3 O3A Cs4A 103(4) . 4_566 ?
O1 Cs1 N31 62.87(17) . . ?
O1 Cs1 N24 90.80(18) . 2_645 ?
N31 Cs1 N24 71.86(12) . 2_645 ?
O1 Cs1 N32 147.3(2) . . ?
N31 Cs1 N32 85.31(13) . . ?
N24 Cs1 N32 71.27(13) 2_645 . ?
O1 Cs1 N42 109.6(2) . . ?
N31 Cs1 N42 140.0(2) . . ?
N24 Cs1 N42 69.0(2) 2_645 . ?
N32 Cs1 N42 89.7(2) . . ?
O1 Cs1 O2A 151.3(6) . 1_655 ?
N31 Cs1 O2A 145.6(5) . 1_655 ?
N24 Cs1 O2A 101.6(4) 2_645 1_655 ?
N32 Cs1 O2A 61.1(5) . 1_655 ?
N42 Cs1 O2A 53.5(6) . 1_655 ?
O1 Cs1 N22 100.2(2) . 4_565 ?
```

```
N31 Cs1 N22 68.45(14) . 4_565 ?
N24 Cs1 N22 127.43(13) 2_645 4_565 ?
N32 Cs1 N22 72.45(13) . 4_565 ?
N42 Cs1 N22 146.2(2) . 4_565 ?
O2A Cs1 N22 92.7(5) 1_655 4_565 ?
O1 Cs1 C31 81.72(18) . . ?
N31 Cs1 C31 19.13(11) . . ?
N24 Cs1 C31 66.08(11) 2_645 . ?
N32 Cs1 C31 66.20(13) . . ?
N42 Cs1 C31 133.8(2) . . ?
O2A Cs1 C31 126.9(5) 1_655 . ?
N22 Cs1 C31 65.04(13) 4_565 . ?
O1 Cs1 O2 164.3(3) . . ?
N31 Cs1 O2 132.3(3) . . ?
N24 Cs1 O2 98.1(3) 2_645 . ?
N32 Cs1 O2 48.4(3) . . ?
N42 Cs1 O2 62.5(3) . . ?
O2A Cs1 O2 13.3(5) 1_655 . ?
N22 Cs1 O2 84.6(3) 4_565 . ?
C31 Cs1 O2 113.7(3) . . ?
O1 Cs1 C32 128.60(19) . . ?
N31 Cs1 C32 66.38(13) . . ?
N24 Cs1 C32 65.87(12) 2_645 . ?
N32 Cs1 C32 18.94(13) . . ?
N42 Cs1 C32 103.64(19) . . ?
O2A Cs1 C32 80.0(5) 1_655 . ?
N22 Cs1 C32 67.38(12) 4_565 . ?
C31 Cs1 C32 47.27(12) . . ?
O2 Cs1 C32 67.1(3) . . ?
O1 Cs1 Pt1 74.50(15) . . ?
N31 Cs1 Pt1 125.51(13) . . ?
N24 Cs1 Pt1 143.27(12) 2_645 . ?
N32 Cs1 Pt1 135.29(11) . . ?
N42 Cs1 Pt1 84.24(19) . . ?
O2A Cs1 Pt1 80.3(5) 1_655 . ?
N22 Cs1 Pt1 88.72(9) 4_565 . ?
C31 Cs1 Pt1 140.72(14) . . ?
O2 Cs1 Pt1 90.8(3) . . ?
C32 Cs1 Pt1 148.08(9) . . ?
O1 Cs1 C14 58.86(19) . . ?
N31 Cs1 C14 95.03(15) . . ?
N24 Cs1 C14 149.39(13) 2_645 . ?
N32 Cs1 C14 136.67(15) . . ?
N42 Cs1 C14 114.83(19) . . ?
O2A Cs1 C14 104.2(4) 1_655 . ?
N22 Cs1 C14 67.62(13) 4_565 . ?
C31 Cs1 C14 109.28(16) . . ?
O2 Cs1 C14 110.6(3) . . ?
C32 Cs1 C14 134.95(16) . . ?
Pt1 Cs1 C14 31.43(8) . . ?
N42 Cs1A O2A 58.6(6) . 1_655 ?
N42 Cs1A N24 74.0(3) . 2_645 ?
O2A Cs1A N24 108.5(6) 1_655 2_645 ?
N42 Cs1A O1 113.6(3) . . ?
O2A Cs1A O1 155.6(6) 1_655 . ?
N24 Cs1A O1 89.3(3) 2_645 . ?
N42 Cs1A N32 95.9(4) . . ?
```

```
O2A Cs1A N32 63.7(6) 1_655 . ?
N24 Cs1A N32 72.55(18) 2_645 . ?
O1 Cs1A N32 139.8(4) . . ?
N42 Cs1A O2 67.9(4) . . ?
O2A Cs1A O2 14.1(5) 1_655 . ?
N24 Cs1A O2 103.6(4) 2_645 . ?
O1 Cs1A O2 166.7(4) . . ?
N32 Cs1A O2 50.0(3) . . ?
N42 Cs1A C42 18.8(2) . . ?
O2A Cs1A C42 75.3(7) 1_655 . ?
N24 Cs1A C42 73.4(3) 2_645 . ?
O1 Cs1A C42 94.8(3) . . ?
N32 Cs1A C42 112.9(4) . . ?
O2 Cs1A C42 86.0(4) . . ?
N42 Cs1A N31 142.4(3) . . ?
O2A Cs1A N31 143.0(6) 1_655 . ?
N24 Cs1A N31 69.43(19) 2_645 . ?
O1 Cs1A N31 58.4(2) . . ?
N32 Cs1A N31 81.5(2) . . ?
O2 Cs1A N31 129.1(4) . . ?
C42 Cs1A N31 133.5(3) . . ?
N42 Cs1A Pt1 89.3(3) . . ?
O2A Cs1A Pt1 83.6(5) 1_655 . ?
N24 Cs1A Pt1 148.6(3) 2_645 . ?
O1 Cs1A Pt1 72.8(2) . . ?
N32 Cs1A Pt1 136.9(2) . . ?
O2 Cs1A Pt1 94.1(3) . . ?
C42 Cs1A Pt1 82.3(2) . . ?
N31 Cs1A Pt1 118.1(3) . . ?
N42 Cs1A C32 109.2(3) . . ?
O2A Cs1A C32 82.0(6) 1_655 . ?
N24 Cs1A C32 65.89(16) 2_645 . ?
O1 Cs1A C32 121.3(4) . . ?
N32 Cs1A C32 18.51(13) . . ?
O2 Cs1A C32 68.2(3) . . ?
C42 Cs1A C32 123.4(3) . . ?
N31 Cs1A C32 63.07(19) . . ?
Pt1 Cs1A C32 145.6(3) . . ?
N42 Cs1A N22 150.6(4) . 4_565 ?
O2A Cs1A N22 92.0(6) 1_655 4_565 ?
N24 Cs1A N22 122.0(3) 2_645 4_565 ?
O1 Cs1A N22 92.4(4) . 4_565 ?
N32 Cs1A N22 69.6(2) . 4_565 ?
O2 Cs1A N22 83.6(3) . 4_565 ?
C42 Cs1A N22 163.1(3) . 4_565 ?
N31 Cs1A N22 62.9(2) . 4_565 ?
Pt1 Cs1A N22 85.2(2) . 4_565 ?
C32 Cs1A N22 64.21(19) . 4_565 ?
N42 Cs1A C31 137.0(3) . . ?
O2A Cs1A C31 126.3(6) 1_655 . ?
N24 Cs1A C31 64.04(17) 2_645 . ?
O1 Cs1A C31 76.1(3) . . ?
N32 Cs1A C31 63.70(18) . . ?
O2 Cs1A C31 112.3(3) . . ?
C42 Cs1A C31 136.4(3) . . ?
N31 Cs1A C31 17.89(12) . . ?
Pt1 Cs1A C31 132.0(4) . . ?
```

```
C32 Cs1A C31 45.22(15) . . ?
N22 Cs1A C31 60.3(2) 4_565 . ?
Cs2A Cs2 N13 108.52(19) . . ?
Cs2A Cs2 N12 135.17(18) . 4_565 ?
N13 Cs2 N12 98.23(19) . 4_565 ?
Cs2A Cs2 O1 43.2(2) . 1_655 ?
N13 Cs2 O1 145.0(2) . 1_655 ?
N12 Cs2 O1 116.6(2) 4_565 1_655 ?
Cs2A Cs2 O2 36.2(3) . . ?
N13 Cs2 O2 75.9(3) . . ?
N12 Cs2 O2 159.0(2) 4_565 . ?
O1 Cs2 O2 70.1(3) 1_655 . ?
Cs2A Cs2 N14 109.51(17) . 1_655 ?
N13 Cs2 N14 132.70(17) . 1_655 ?
N12 Cs2 N14 73.01(16) 4_565 1_655 ?
O1 Cs2 N14 66.4(2) 1_655 1_655 ?
O2 Cs2 N14 125.8(2) . 1_655 ?
Cs2A Cs2 N23 140.09(16) . 1_655 ?
N13 Cs2 N23 64.07(15) . 1_655 ?
N12 Cs2 N23 83.87(14) 4_565 1_655 ?
O1 Cs2 N23 120.59(18) 1_655 1_655 ?
O2 Cs2 N23 110.5(3) . 1_655 ?
N14 Cs2 N23 68.76(13) 1_655 1_655 ?
Cs2A Cs2 N22 84.38(15) . 4_565 ?
N13 Cs2 N22 69.96(13) . 4_565 ?
N12 Cs2 N22 71.64(14) 4_565 4_565 ?
O1 Cs2 N22 116.01(17) 1_655 4_565 ?
O2 Cs2 N22 87.5(2) . 4_565 ?
N14 Cs2 N22 140.53(12) 1_655 4_565 ?
N23 Cs2 N22 123.40(11) 1_655 4_565 ?
Cs2A Cs2 N11 69.20(16) . 1_655 ?
N13 Cs2 N11 85.30(15) . 1_655 ?
N12 Cs2 N11 150.25(14) 4_565 1_655 ?
O1 Cs2 N11 66.59(17) 1_655 1_655 ?
O2 Cs2 N11 50.4(2) . 1_655 ?
N14 Cs2 N11 82.88(14) 1_655 1_655 ?
N23 Cs2 N11 71.08(13) 1_655 1_655 ?
N22 Cs2 N11 135.86(13) 4_565 1_655 ?
Cs2A Cs2 N21 61.62(15) . 4_565 ?
N13 Cs2 N21 146.66(13) . 4_565 ?
N12 Cs2 N21 76.16(15) 4_565 4_565 ?
O1 Cs2 N21 49.67(16) 1_655 4_565 ?
O2 Cs2 N21 97.5(3) . 4_565 ?
N14 Cs2 N21 77.83(12) 1_655 4_565 ?
N23 Cs2 N21 144.88(11) 1_655 4_565 ?
N22 Cs2 N21 77.19(11) 4_565 4_565 ?
N11 Cs2 N21 115.98(13) 1_655 4_565 ?
Cs2A Cs2 C14 100.57(16) . 1_655 ?
N13 Cs2 C14 126.28(14) . 1_655 ?
N12 Cs2 C14 91.04(16) 4_565 1_655 ?
O1 Cs2 C14 60.28(19) 1_655 1_655 ?
O2 Cs2 C14 108.8(2) . 1_655 ?
N14 Cs2 C14 18.77(14) 1_655 1_655 ?
N23 Cs2 C14 64.58(12) 1_655 1_655 ?
N22 Cs2 C14 158.75(12) 4_565 1_655 ?
N11 Cs2 C14 64.11(14) 1_655 1_655 ?
N21 Cs2 C14 86.95(11) 4_565 1_655 ?
```

```
Cs2A Cs2 C11 77.33(16) . 1_655 ?
N13 Cs2 C11 97.91(14) . 1_655 ?
N12 Cs2 C11 134.44(15) 4_565 1_655 ?
O1 Cs2 C11 60.82(17) 1_655 1_655 ?
O2 Cs2 C11 66.5(2) . 1_655 ?
N14 Cs2 C11 64.79(14) 1_655 1_655 ?
N23 Cs2 C11 65.86(12) 1_655 1_655 ?
N22 Cs2 C11 153.62(13) 4_565 1_655 ?
N11 Cs2 C11 18.09(14) 1_655 1_655 ?
N21 Cs2 C11 109.48(12) 4_565 1_655 ?
C14 Cs2 C11 46.02(14) 1_655 1_655 ?
Cs2 Cs2A O1 126.5(2) . 1_655 ?
Cs2 Cs2A O2 134.9(4) . . ?
O1 Cs2A O2 86.1(4) 1_655 . ?
Cs2 Cs2A O2A 124.0(5) . 1_655 ?
O1 Cs2A O2A 96.3(5) 1_655 1_655 ?
O2 Cs2A O2A 11.2(5) . 1_655 ?
Cs2 Cs2A N21 107.29(17) . 4_565 ?
O1 Cs2A N21 55.94(19) 1_655 4_565 ?
O2 Cs2A N21 117.4(3) . 4_565 ?
O2A Cs2A N21 127.6(5) 1_655 4_565 ?
Cs2 Cs2A N11 99.12(17) . 1_655 ?
O1 Cs2A N11 74.6(2) 1_655 1_655 ?
O2 Cs2A N11 56.2(3) . 1_655 ?
O2A Cs2A N11 55.2(4) 1_655 1_655 ?
N21 Cs2A N11 130.44(15) 4_565 1_655 ?
Cs2 Cs2A N32 155.24(18) . . ?
O1 Cs2A N32 71.8(2) 1_655 . ?
O2 Cs2A N32 53.7(3) . . ?
O2A Cs2A N32 61.9(5) 1_655 . ?
N21 Cs2A N32 67.01(13) 4_565 . ?
N11 Cs2A N32 102.37(15) 1_655 . ?
Cs2 Cs2A N22 83.56(15) . 4_565 ?
O1 Cs2A N22 131.7(2) 1_655 4_565 ?
O2 Cs2A N22 97.0(3) . 4_565 ?
O2A Cs2A N22 93.6(4) 1_655 4_565 ?
N21 Cs2A N22 81.00(12) 4_565 4_565 ?
N11 Cs2A N22 144.22(14) 1_655 4_565 ?
N32 Cs2A N22 71.82(13) . 4_565 ?
Cs2 Cs2A N13 60.13(17) . . ?
O1 Cs2A N13 158.0(2) 1_655 . ?
O2 Cs2A N13 78.6(3) . . ?
O2A Cs2A N13 67.6(5) 1_655 . ?
N21 Cs2A N13 145.82(14) 4_565 . ?
N11 Cs2A N13 83.73(15) 1_655 . ?
N32 Cs2A N13 110.14(16) . . ?
N22 Cs2A N13 66.60(12) 4_565 . ?
Cs2 Cs2A C11 91.43(16) . 1_655 ?
O1 Cs2A C11 65.8(2) 1_655 1_655 ?
O2 Cs2A C11 73.2(3) . 1_655 ?
O2A Cs2A C11 73.4(4) 1_655 1_655 ?
N21 Cs2A C11 118.64(14) 4_565 1_655 ?
N11 Cs2A C11 18.49(15) 1_655 1_655 ?
N32 Cs2A C11 112.65(14) . 1_655 ?
N22 Cs2A C11 160.28(13) 4_565 1_655 ?
N13 Cs2A C11 94.36(14) . 1_655 ?
Cs2 Cs2A C21 103.26(16) . 4_565 ?
```

```
O1 Cs2A C21 73.15(19) 1_655 4_565 ?
O2 Cs2A C21 117.0(3) . 4_565 ?
O2A Cs2A C21 124.7(5) 1_655 4_565 ?
N21 Cs2A C21 18.41(12) 4_565 4_565 ?
N11 Cs2A C21 147.45(15) 1_655 4_565 ?
N32 Cs2A C21 63.32(13) . 4_565 ?
N22 Cs2A C21 62.59(11) 4_565 4_565 ?
N13 Cs2A C21 128.04(13) . 4_565 ?
C11 Cs2A C21 137.05(14) 1_655 4_565 ?
Cs2 Cs2A N14 59.80(16) . 1_655 ?
O1 Cs2A N14 66.7(2) 1_655 1_655 ?
O2 Cs2A N14 134.6(3) . 1_655 ?
O2A Cs2A N14 136.2(4) 1_655 1_655 ?
N21 Cs2A N14 77.39(12) 4_565 1_655 ?
N11 Cs2A N14 81.08(14) 1_655 1_655 ?
N32 Cs2A N14 135.81(14) . 1_655 ?
N22 Cs2A N14 128.34(13) 4_565 1_655 ?
N13 Cs2A N14 114.01(16) . 1_655 ?
C11 Cs2A N14 62.85(14) 1_655 1_655 ?
C21 Cs2A N14 90.04(12) 4_565 1_655 ?
N21 Cs3 N14 88.00(15) 1_455 4_566 ?
N21 Cs3 O3 117.2(3) 1_455 . ?
N14 Cs3 O3 67.7(5) 4_566 . ?
N21 Cs3 N13 78.88(15) 1_455 1_455 ?
N14 Cs3 N13 137.5(2) 4_566 1_455 ?
O3 Cs3 N13 82.7(5) . 1_455 ?
N21 Cs3 N23 103.98(15) 1_455 . ?
N14 Cs3 N23 158.16(16) 4_566 . ?
O3 Cs3 N23 119.9(4) . . ?
N13 Cs3 N23 63.81(15) 1_455 . ?
N21 Cs3 N22 122.33(17) 1_455 . ?
N14 Cs3 N22 72.72(13) 4_566 . ?
O3 Cs3 N22 104.7(3) . . ?
N13 Cs3 N22 147.09(14) 1_455 . ?
N23 Cs3 N22 85.44(13) . . ?
N21 Cs3 N11 164.56(18) 1_455 . ?
N14 Cs3 N11 99.65(18) 4_566 . ?
O3 Cs3 N11 55.2(3) . . ?
N13 Cs3 N11 86.50(17) 1_455 . ?
N23 Cs3 N11 73.42(14) . . ?
N22 Cs3 N11 72.97(13) . . ?
N21 Cs3 N31 63.30(14) 1_455 4_566 ?
N14 Cs3 N31 98.54(17) 4_566 4_566 ?
O3 Cs3 N31 165.9(5) . 4_566 ?
N13 Cs3 N31 110.66(18) 1_455 4_566 ?
N23 Cs3 N31 71.77(14) . 4_566 ?
N22 Cs3 N31 66.67(14) . 4_566 ?
N11 Cs3 N31 127.81(16) . 4_566 ?
N21 Cs3 C23 113.63(17) 1_455 . ?
N14 Cs3 C23 139.20(15) 4_566 . ?
O3 Cs3 C23 122.5(4) . . ?
N13 Cs3 C23 82.34(14) 1_455 . ?
N23 Cs3 C23 18.97(11) . . ?
N22 Cs3 C23 66.48(12) . . ?
N11 Cs3 C23 68.72(13) . . ?
N31 Cs3 C23 65.66(13) 4_566 . ?
N21 Cs3 C22 125.24(19) 1_455 . ?
```

```
N14 Cs3 C22 91.59(13) 4_566 . ?
O3 Cs3 C22 112.9(3) . . ?
N13 Cs3 C22 128.91(15) 1_455 . ?
N23 Cs3 C22 66.58(13) . . ?
N22 Cs3 C22 18.87(11) . . ?
N11 Cs3 C22 68.33(13) . . ?
N31 Cs3 C22 62.67(13) 4_566 . ?
C23 Cs3 C22 47.61(12) . . ?
N21 Cs3 C13 70.56(13) 1_455 1_455 ?
N14 Cs3 C13 119.72(18) 4_566 1_455 ?
O3 Cs3 C13 73.8(4) . 1_455 ?
N13 Cs3 C13 18.14(16) 1_455 1_455 ?
N23 Cs3 C13 81.81(14) . 1_455 ?
N22 Cs3 C13 163.98(12) . 1_455 ?
N11 Cs3 C13 94.01(16) . 1_455 ?
N31 Cs3 C13 117.70(15) 4_566 1_455 ?
C23 Cs3 C13 100.45(13) . 1_455 ?
C22 Cs3 C13 146.84(13) . 1_455 ?
N21 Cs3 O3A 116.7(14) 1_455 . ?
N14 Cs3 O3A 80(2) 4_566 . ?
O3 Cs3 O3A 13(2) . . ?
N13 Cs3 O3A 70(2) 1_455 . ?
N23 Cs3 O3A 109(2) . . ?
N22 Cs3 O3A 112.8(15) . . ?
N11 Cs3 O3A 52.5(16) . . ?
N31 Cs3 O3A 179(3) 4_566 . ?
C23 Cs3 O3A 115(2) . . ?
C22 Cs3 O3A 117.2(14) . . ?
C13 Cs3 O3A 63.1(19) 1_455 . ?
O3 Cs3A N14 72.3(6) . 4_566 ?
O3 Cs3A N13 89.6(6) . 1_455 ?
N14 Cs3A N13 145.9(5) 4_566 1_455 ?
O3 Cs3A N21 123.8(5) . 1_455 ?
N14 Cs3A N21 87.3(2) 4_566 1_455 ?
N13 Cs3A N21 79.0(2) 1_455 1_455 ?
O3 Cs3A N11 59.2(4) . . ?
N14 Cs3A N11 103.7(3) 4_566 . ?
N13 Cs3A N11 90.4(3) 1_455 . ?
N21 Cs3A N11 168.8(3) 1_455 . ?
O3 Cs3A O3A 14(2) . . ?
N14 Cs3A O3A 86(3) 4_566 . ?
N13 Cs3A O3A 76(2) 1_455 . ?
N21 Cs3A O3A 123.2(16) 1_455 . ?
N11 Cs3A O3A 56.4(17) . . ?
O3 Cs3A N23 124.5(6) . . ?
N14 Cs3A N23 150.7(5) 4_566 . ?
N13 Cs3A N23 63.0(2) 1_455 . ?
N21 Cs3A N23 98.6(3) 1_455 . ?
N11 Cs3A N23 72.97(19) . . ?
O3A Cs3A N23 113(3) . . ?
O3 Cs3A C13 79.9(6) . 1_455 ?
N14 Cs3A C13 126.7(4) 4_566 1_455 ?
N13 Cs3A C13 19.20(17) 1_455 1_455 ?
N21 Cs3A C13 71.68(19) 1_455 1_455 ?
N11 Cs3A C13 99.4(3) . 1_455 ?
O3A Cs3A C13 68(2) . 1_455 ?
N23 Cs3A C13 82.04(19) . 1_455 ?
```

```
O3 Cs3A N22 107.4(4) . . ?
N14 Cs3A N22 70.9(2) 4_566 . ?
N13 Cs3A N22 143.1(3) 1_455 . ?
N21 Cs3A N22 114.4(4) 1_455 . ?
N11 Cs3A N22 72.21(19) . . ?
O3A Cs3A N22 116.3(17) . . ?
N23 Cs3A N22 80.6(3) . . ?
C13 Cs3A N22 162.3(3) 1_455 . ?
O3 Cs3A C23 125.7(5) . . ?
N14 Cs3A C23 133.4(4) 4_566 . ?
N13 Cs3A C23 80.7(2) 1_455 . ?
N21 Cs3A C23 106.6(4) 1_455 . ?
N11 Cs3A C23 67.61(19) . . ?
O3A Cs3A C23 118(2) . . ?
N23 Cs3A C23 17.93(12) . . ?
C13 Cs3A C23 99.8(2) 1_455 . ?
N22 Cs3A C23 62.7(2) . . ?
O3 Cs3A N31 164.7(6) . 4_566 ?
N14 Cs3A N31 93.3(3) 4_566 4_566 ?
N13 Cs3A N31 105.5(3) 1_455 4_566 ?
N21 Cs3A N31 58.8(3) 1_455 4_566 ?
N11 Cs3A N31 121.7(4) . 4_566 ?
O3A Cs3A N31 177.9(15) . 4_566 ?
N23 Cs3A N31 66.4(3) . 4_566 ?
C13 Cs3A N31 113.8(3) 1_455 4_566 ?
N22 Cs3A N31 61.6(3) . 4_566 ?
C23 Cs3A N31 60.8(3) . 4_566 ?
O3 Cs3A C22 115.1(4) . . ?
N14 Cs3A C22 88.7(2) 4_566 . ?
N13 Cs3A C22 125.3(3) 1_455 . ?
N21 Cs3A C22 116.2(5) 1_455 . ?
N11 Cs3A C22 67.05(19) . . ?
O3A Cs3A C22 119.9(15) . . ?
N23 Cs3A C22 62.8(2) . . ?
C13 Cs3A C22 144.5(3) 1_455 . ?
N22 Cs3A C22 17.80(12) . . ?
C23 Cs3A C22 44.95(18) . . ?
N31 Cs3A C22 58.0(2) 4_566 . ?
Cs4A Cs4 O3 129.8(5) . 4_565 ?
Cs4A Cs4 N12 117.5(2) . 4_465 ?
O3 Cs4 N12 63.6(3) 4_565 4_465 ?
Cs4A Cs4 N23 99.4(2) . . ?
O3 Cs4 N23 129.1(4) 4_565 . ?
N12 Cs4 N23 84.31(14) 4_465 . ?
Cs4A Cs4 N42 78.4(3) . 2_655 ?
O3 Cs4 N42 67.1(4) 4_565 2_655 ?
N12 Cs4 N42 125.2(2) 4_465 2_655 ?
N23 Cs4 N42 148.16(16) . 2_655 ?
Cs4A Cs4 N24 103.6(2) . . ?
O3 Cs4 N24 96.4(4) 4_565 . ?
N12 Cs4 N24 138.22(16) 4_465 . ?
N23 Cs4 N24 81.71(11) . . ?
N42 Cs4 N24 68.28(17) 2_655 . ?
Cs4A Cs4 N32 43.1(2) . 2_655 ?
O3 Cs4 N32 155.5(3) 4_565 2_655 ?
N12 Cs4 N32 140.06(16) 4_465 2_655 ?
N23 Cs4 N32 69.90(13) . 2_655 ?
```

```
N42 Cs4 N32 88.9(2) 2_655 2_655 ?
N24 Cs4 N32 68.93(12) . 2_655 ?
Cs4A Cs4 O3A 117(2) . 4_565 ?
O3 Cs4 O3A 13.8(17) 4_565 4_565 ?
N12 Cs4 O3A 63.2(15) 4_465 4_565 ?
N23 Cs4 O3A 139.3(18) . 4_565 ?
N42 Cs4 O3A 63.1(16) 2_655 4_565 ?
N24 Cs4 O3A 105.8(16) . 4_565 ?
N32 Cs4 O3A 150.5(17) 2_655 4_565 ?
Cs4A Cs4 N41 40.2(3) . 2 ?
O3 Cs4 N41 131.4(4) 4_565 2 ?
N12 Cs4 N41 82.7(2) 4_465 2 ?
N23 Cs4 N41 76.29(18) . 2 ?
N42 Cs4 N41 115.4(3) 2_655 2 ?
N24 Cs4 N41 130.82(18) . 2 ?
N32 Cs4 N41 62.3(2) 2_655 2 ?
O3A Cs4 N41 119.6(18) 4_565 2 ?
Cs4A Cs4 N14 164.6(2) . . ?
O3 Cs4 N14 65.2(5) 4_565 . ?
N12 Cs4 N14 70.20(16) 4_465 . ?
N23 Cs4 N14 67.17(12) . . ?
N42 Cs4 N14 108.7(3) 2_655 . ?
N24 Cs4 N14 68.08(12) . . ?
N32 Cs4 N14 122.08(13) 2_655 . ?
O3A Cs4 N14 79(2) 4_565 . ?
N41 Cs4 N14 135.8(2) 2 . ?
Cs4A Cs4 C23 102.7(2) . . ?
O3 Cs4 C23 127.3(5) 4_565 . ?
N12 Cs4 C23 98.57(14) 4_465 . ?
N23 Cs4 C23 18.36(11) . . ?
N42 Cs4 C23 130.48(16) 2_655 . ?
N24 Cs4 C23 63.35(11) . . ?
N32 Cs4 C23 64.76(12) 2_655 . ?
O3A Cs4 C23 141(2) 4_565 . ?
N41 Cs4 C23 89.58(16) 2 . ?
N14 Cs4 C23 62.12(11) . . ?
Cs4A Cs4 O2 17.7(3) . 2_655 ?
O3 Cs4 O2 118.7(5) 4_565 2_655 ?
N12 Cs4 O2 128.7(2) 4_465 2_655 ?
N23 Cs4 O2 112.2(3) . 2_655 ?
N42 Cs4 O2 61.0(3) 2_655 2_655 ?
N24 Cs4 O2 93.0(2) . 2_655 ?
N32 Cs4 O2 46.3(3) 2_655 2_655 ?
O3A Cs4 O2 107.3(19) 4_565 2_655 ?
N41 Cs4 O2 57.6(3) 2 2_655 ?
N14 Cs4 O2 161.0(2) . 2_655 ?
C23 Cs4 O2 110.9(3) . 2_655 ?
Cs4 Cs4A N32 129.1(2) . 2_655 ?
Cs4 Cs4A N41 132.4(4) . 2 ?
N32 Cs4A N41 72.3(2) 2_655 2 ?
Cs4 Cs4A O2 158.9(4) . 2_655 ?
N32 Cs4A O2 54.5(3) 2_655 2_655 ?
N41 Cs4A O2 68.2(4) 2 2_655 ?
Cs4 Cs4A N42 91.2(3) . 2_655 ?
N32 Cs4A N42 97.8(2) 2_655 2_655 ?
N41 Cs4A N42 131.7(4) 2 2_655 ?
O2 Cs4A N42 68.1(4) 2_655 2_655 ?
```

```
Cs4 Cs4A O2A 146.1(6) . 2 ?
N32 Cs4A O2A 65.0(5) 2_655 2 ?
N41 Cs4A O2A 79.1(5) 2 2 ?
O2 Cs4A O2A 13.9(5) 2_655 2 ?
N42 Cs4A O2A 55.0(6) 2_655 2 ?
Cs4 Cs4A O3 42.2(5) . 4_565 ?
N32 Cs4A O3 155.1(3) 2_655 4_565 ?
N41 Cs4A O3 132.2(4) 2 4_565 ?
O2 Cs4A O3 123.8(5) 2_655 4_565 ?
N42 Cs4A O3 63.4(4) 2_655 4_565 ?
O2A Cs4A O3 110.2(6) 2 4_565 ?
Cs4 Cs4A C41 127.5(3) . 2 ?
N32 Cs4A C41 89.0(2) 2_655 2 ?
N41 Cs4A C41 19.3(2) 2 2 ?
O2 Cs4A C41 69.9(3) 2_655 2 ?
N42 Cs4A C41 121.5(3) 2_655 2 ?
O2A Cs4A C41 77.2(4) 2 2 ?
O3 Cs4A C41 114.4(4) 4_565 2 ?
Cs4 Cs4A N23 70.8(2) . . ?
N32 Cs4A N23 72.81(14) 2_655 . ?
N41 Cs4A N23 80.0(2) 2 . ?
O2 Cs4A N23 124.1(3) 2_655 . ?
N42 Cs4A N23 143.6(2) 2_655 . ?
O2A Cs4A N23 136.9(6) 2 . ?
O3 Cs4A N23 111.8(4) 4_565 . ?
C41 Cs4A N23 93.98(17) 2 . ?
Cs4 Cs4A N12 53.8(2) . 4_465 ?
N32 Cs4A N12 144.70(17) 2_655 4_465 ?
N41 Cs4A N12 84.2(3) 2 4_465 ?
O2 Cs4A N12 138.6(3) 2_655 4_465 ?
N42 Cs4A N12 117.5(2) 2_655 4_465 ?
O2A Cs4A N12 136.5(5) 2 4_465 ?
O3 Cs4A N12 56.2(3) 4_565 4_465 ?
C41 Cs4A N12 74.2(2) 2 4_465 ?
N23 Cs4A N12 77.57(14) . 4_465 ?
Cs4 Cs4A N42 97.7(3) . 4_465 ?
N32 Cs4A N42 132.6(3) 2_655 4_465 ?
N41 Cs4A N42 82.3(3) 2 4_465 ?
O2 Cs4A N42 79.3(3) 2_655 4_465 ?
N42 Cs4A N42 70.4(2) 2_655 4_465 ?
O2A Cs4A N42 71.4(5) 2 4_465 ?
O3 Cs4A N42 59.3(5) 4_565 4_465 ?
C41 Cs4A N42 63.3(2) 2 4_465 ?
N23 Cs4A N42 141.32(18) . 4_465 ?
N12 Cs4A N42 66.6(2) 4_465 4_465 ?
Cs4 Cs4A N24 67.1(2) . . ?
N32 Cs4A N24 70.95(13) 2_655 . ?
N41 Cs4A N24 140.94(19) 2 . ?
O2 Cs4A N24 99.8(2) 2_655 . ?
N42 Cs4A N24 66.70(18) 2_655 . ?
O2A Cs4A N24 96.8(4) 2 . ?
O3 Cs4A N24 86.0(4) 4_565 . ?
C41 Cs4A N24 159.67(19) 2 . ?
N23 Cs4A N24 77.05(12) . . ?
N12 Cs4A N24 120.44(16) 4_465 . ?
N42 Cs4A N24 133.69(19) 4_465 . ?
Cs5A Cs5 N41 73.7(3) . 2_655 ?
```

```
Cs5A Cs5 N23 109.2(2) . 1_655 ?
N41 Cs5 N23 84.1(3) 2_655 1_655 ?
Cs5A Cs5 N31 77.7(2) . 4_666 ?
N41 Cs5 N31 137.88(18) 2_655 4_666 ?
N23 Cs5 N31 76.82(12) 1_655 4_666 ?
Cs5A Cs5 N21 121.0(2) . . ?
N41 Cs5 N21 158.08(19) 2_655 . ?
N23 Cs5 N21 103.80(12) 1_655 . ?
N31 Cs5 N21 63.99(12) 4_666 . ?
Cs5A Cs5 N31 63.5(2) . 2_655 ?
N41 Cs5 N31 101.4(3) 2_655 2_655 ?
N23 Cs5 N31 168.58(12) 1_655 2_655 ?
N31 Cs5 N31 92.66(12) 4_666 2_655 ?
N21 Cs5 N31 74.86(12) . 2_655 ?
Cs5A Cs5 N24 115.3(2) . . ?
N41 Cs5 N24 73.73(19) 2_655 . ?
N23 Cs5 N24 120.93(12) 1_655 . ?
N31 Cs5 N24 147.80(12) 4_666 . ?
N21 Cs5 N24 84.81(12) . . ?
N31 Cs5 N24 70.43(11) 2_655 . ?
Cs5A Cs5 O1 32.5(2) . 2_655 ?
N41 Cs5 O1 50.5(3) 2_655 2_655 ?
N23 Cs5 O1 120.45(16) 1_655 2_655 ?
N31 Cs5 O1 109.94(16) 4_666 2_655 ?
N21 Cs5 O1 133.20(16) . 2_655 ?
N31 Cs5 O1 58.70(16) 2_655 2_655 ?
N24 Cs5 O1 85.05(15) . 2_655 ?
Cs5A Cs5 C21 128.0(2) . . ?
N41 Cs5 C21 139.28(19) 2_655 . ?
N23 Cs5 C21 112.40(12) 1_655 . ?
N31 Cs5 C21 82.84(12) 4_666 . ?
N21 Cs5 C21 18.97(12) . . ?
N31 Cs5 C21 69.94(11) 2_655 . ?
N24 Cs5 C21 65.84(12) . . ?
O1 Cs5 C21 127.11(16) 2_655 . ?
Cs5A Cs5 C24 124.5(2) . . ?
N41 Cs5 C24 92.59(19) 2_655 . ?
N23 Cs5 C24 122.80(12) 1_655 . ?
N31 Cs5 C24 129.30(11) 4_666 . ?
N21 Cs5 C24 65.86(12) . . ?
N31 Cs5 C24 67.39(11) 2_655 . ?
N24 Cs5 C24 18.96(11) . . ?
O1 Cs5 C24 98.63(16) 2_655 . ?
C21 Cs5 C24 46.89(11) . . ?
Cs5A Cs5 C31 67.1(2) . 4_666 ?
N41 Cs5 C31 120.11(18) 2_655 4_666 ?
N23 Cs5 C31 69.11(12) 1_655 4_666 ?
N31 Cs5 C31 17.79(11) 4_666 4_666 ?
N21 Cs5 C31 81.71(11) . 4_666 ?
N31 Cs5 C31 99.54(11) 2_655 4_666 ?
N24 Cs5 C31 165.00(11) . 4_666 ?
O1 Cs5 C31 99.42(15) 2_655 4_666 ?
C21 Cs5 C31 100.60(11) . 4_666 ?
C24 Cs5 C31 147.03(11) . 4_666 ?
Cs5A Cs5 N13 167.2(2) . . ?
N41 Cs5 N13 96.5(3) 2_655 . ?
N23 Cs5 N13 60.61(13) 1_655 . ?
```

```
N31 Cs5 N13 105.75(13) 4_666 . ?
N21 Cs5 N13 70.86(14) . . ?
N31 Cs5 N13 127.83(13) 2_655 . ?
N24 Cs5 N13 68.42(12) . . ?
O1 Cs5 N13 143.42(16) 2_655 . ?
C21 Cs5 N13 64.79(13) . . ?
C24 Cs5 N13 63.17(12) . . ?
C31 Cs5 N13 112.76(12) 4_666 . ?
Cs5 Cs5A N41 96.4(3) . 2_655 ?
Cs5 Cs5A O1 142.0(3) . 2_655 ?
N41 Cs5A O1 55.9(4) 2_655 2_655 ?
Cs5 Cs5A N31 107.7(2) . 2_655 ?
N41 Cs5A N31 108.7(3) 2_655 2_655 ?
O1 Cs5A N31 65.54(18) 2_655 2_655 ?
Cs5 Cs5A N31 92.7(2) . 4_666 ?
N41 Cs5A N31 147.4(2) 2_655 4_666 ?
O1 Cs5A N31 124.84(18) 2_655 4_666 ?
N31 Cs5A N31 98.01(12) 2_655 4_666 ?
Cs5 Cs5A N23 62.2(2) . 1_655 ?
N41 Cs5A N23 82.1(3) 2_655 1_655 ?
O1 Cs5A N23 127.85(18) 2_655 1_655 ?
N31 Cs5A N23 166.61(13) 2_655 1_655 ?
N31 Cs5A N23 74.74(12) 4_666 1_655 ?
Cs5 Cs5A C31 104.7(2) . 4_666 ?
N41 Cs5A C31 129.5(2) 2_655 4_666 ?
O1 Cs5A C31 112.96(17) 2_655 4_666 ?
N31 Cs5A C31 107.57(12) 2_655 4_666 ?
N31 Cs5A C31 19.07(11) 4_666 4_666 ?
N23 Cs5A C31 69.04(12) 1_655 4_666 ?
Cs5 Cs5A N32 129.8(2) . 2_755 ?
N41 Cs5A N32 66.46(19) 2_655 2_755 ?
O1 Cs5A N32 66.96(18) 2_655 2_755 ?
N31 Cs5A N32 122.41(13) 2_655 2_755 ?
N31 Cs5A N32 83.78(13) 4_666 2_755 ?
N23 Cs5A N32 68.68(13) 1_655 2_755 ?
C31 Cs5A N32 64.71(12) 4_666 2_755 ?
Cs5 Cs5A N21 161.2(2) . 3_766 ?
N41 Cs5A N21 102.0(3) 2_655 3_766 ?
O1 Cs5A N21 51.29(17) 2_655 3_766 ?
N31 Cs5A N21 62.25(12) 2_655 3_766 ?
N31 Cs5A N21 74.07(12) 4_666 3_766 ?
N23 Cs5A N21 124.45(12) 1_655 3_766 ?
C31 Cs5A N21 66.50(12) 4_666 3_766 ?
N32 Cs5A N21 63.23(12) 2_755 3_766 ?
Cs5 Cs5A N24 57.0(2) . . ?
N41 Cs5A N24 71.10(19) 2_655 . ?
O1 Cs5A N24 87.43(17) 2_655 . ?
N31 Cs5A N24 69.29(12) 2_655 . ?
N31 Cs5A N24 137.90(12) 4_666 . ?
N23 Cs5A N24 108.34(12) 1_655 . ?
C31 Cs5A N24 156.53(12) 4_666 . ?
N32 Cs5A N24 137.49(12) 2_755 . ?
N21 Cs5A N24 125.58(11) 3_766 . ?
Cs5 Cs5A N21 51.7(2) . . ?
N41 Cs5A N21 144.2(2) 2_655 . ?
O1 Cs5A N21 138.65(18) 2_655 . ?
N31 Cs5A N21 73.13(12) 2_655 . ?
```

```
N31 Cs5A N21 61.09(12) 4_666 . ?
N23 Cs5A N21 93.48(12) 1_655 . ?
C31 Cs5A N21 80.02(11) 4_666 . ?
N32 Cs5A N21 144.12(13) 2_755 . ?
N21 Cs5A N21 109.52(11) 3_766 . ?
N24 Cs5A N21 76.84(11) . . ?
Cs5 Cs5A C32 126.9(2) . 2_755 ?
N41 Cs5A C32 84.4(2) 2_655 2_755 ?
O1 Cs5A C32 79.85(18) 2_655 2_755 ?
N31 Cs5A C32 122.36(13) 2_655 2_755 ?
N31 Cs5A C32 65.41(12) 4_666 2_755 ?
N23 Cs5A C32 65.37(12) 1_655 2_755 ?
C31 Cs5A C32 46.34(12) 4_666 2_755 ?
N32 Cs5A C32 18.37(12) 2_755 2_755 ?
N21 Cs5A C32 60.12(11) 3_766 2_755 ?
N24 Cs5A C32 155.42(12) . 2_755 ?
N21 Cs5A C32 125.99(12) . 2_755 ?
N22 Cs6 N24 133.81(13) 4_565 . ?
N22 Cs6 N13 71.72(15) 4_565 . ?
N24 Cs6 N13 75.22(15) . . ?
N22 Cs6 N11 74.96(13) 4_565 4_565 ?
N24 Cs6 N11 131.55(16) . 4_565 ?
N13 Cs6 N11 146.68(17) . 4_565 ?
N22 Cs6 C41 145.9(2) 4_565 2_655 ?
N24 Cs6 C41 76.2(2) . 2_655 ?
N13 Cs6 C41 110.1(2) . 2_655 ?
N11 Cs6 C41 97.17(18) 4_565 2_655 ?
N22 Cs6 N12 71.46(14) 4_565 4_565 ?
N24 Cs6 N12 140.30(15) . 4_565 ?
N13 Cs6 N12 90.53(16) . 4_565 ?
N11 Cs6 N12 78.49(15) 4_565 4_565 ?
C41 Cs6 N12 74.4(2) 2_655 4_565 ?
N22 Cs6 N14 70.57(13) 4_565 . ?
N24 Cs6 N14 71.34(13) . . ?
N13 Cs6 N14 77.22(15) . . ?
N11 Cs6 N14 92.23(15) 4_565 . ?
C41 Cs6 N14 143.5(2) 2_655 . ?
N12 Cs6 N14 142.02(15) 4_565 . ?
N22 Cs6 N41 143.3(3) 4_565 2_655 ?
N24 Cs6 N41 68.0(2) . 2_655 ?
N13 Cs6 N41 92.4(2) . 2_655 ?
N11 Cs6 N41 114.69(17) 4_565 2_655 ?
C41 Cs6 N41 17.92(19) 2_655 2_655 ?
N12 Cs6 N41 76.0(3) 4_565 2_655 ?
N14 Cs6 N41 139.4(2) . 2_655 ?
N22 Cs6 C11 67.69(12) 4_565 4_565 ?
N24 Cs6 C11 147.89(15) . 4_565 ?
N13 Cs6 C11 135.95(16) . 4_565 ?
N11 Cs6 C11 17.75(14) 4_565 4_565 ?
C41 Cs6 C11 94.66(18) 2_655 4_565 ?
N12 Cs6 C11 61.06(14) 4_565 4_565 ?
N14 Cs6 C11 104.05(14) . 4_565 ?
N41 Cs6 C11 110.16(17) 2_655 4_565 ?
N22 Cs6 C13 69.39(13) 4_565 . ?
N24 Cs6 C13 69.32(13) . . ?
N13 Cs6 C13 17.60(14) . . ?
N11 Cs6 C13 140.16(15) 4_565 . ?
```

```
C41 Cs6 C13 122.36(17) 2_655 . ?
N12 Cs6 C13 105.64(15) 4_565 . ?
N14 Cs6 C13 59.72(13) . . ?
N41 Cs6 C13 104.54(17) 2_655 . ?
C11 Cs6 C13 137.08(13) 4_565 . ?
N22 Cs6 C12 65.69(12) 4_565 4_565 ?
N24 Cs6 C12 155.17(14) . 4_565 ?
N13 Cs6 C12 103.47(16) . 4_565 ?
N11 Cs6 C12 61.27(14) 4_565 4_565 ?
C41 Cs6 C12 81.3(2) 2_655 4_565 ?
N12 Cs6 C12 17.52(13) 4_565 4_565 ?
N14 Cs6 C12 133.14(14) . 4_565 ?
N41 Cs6 C12 87.4(2) 2_655 4_565 ?
C11 Cs6 C12 43.68(13) 4_565 4_565 ?
C13 Cs6 C12 116.07(14) . 4_565 ?
N22 Cs6 C14 68.73(12) 4_565 . ?
N24 Cs6 C14 67.06(12) . . ?
N13 Cs6 C14 59.98(14) . . ?
N11 Cs6 C14 107.74(15) 4_565 . ?
C41 Cs6 C14 143.2(2) 2_655 . ?
N12 Cs6 C14 136.07(15) 4_565 . ?
N14 Cs6 C14 17.34(12) . . ?
N41 Cs6 C14 131.79(18) 2_655 . ?
C11 Cs6 C14 117.06(13) 4_565 . ?
C13 Cs6 C14 42.42(13) . . ?
C12 Cs6 C14 134.40(13) 4_565 . ?
N24 Cs6A N22 134.24(17) . 4_565 ?
N24 Cs6A N11 142.87(19) . 4_565 ?
N22 Cs6A N11 76.82(15) 4_565 4_565 ?
N24 Cs6A N14 76.01(15) . . ?
N22 Cs6A N14 73.56(15) 4_565 . ?
N11 Cs6A N14 101.04(18) 4_565 . ?
N24 Cs6A O3 93.4(3) . 4_565 ?
N22 Cs6A O3 102.9(2) 4_565 4_565 ?
N11 Cs6A O3 54.5(4) 4_565 4_565 ?
N14 Cs6A O3 64.1(4) . 4_565 ?
N24 Cs6A N13 72.68(16) . . ?
N22 Cs6A N13 68.03(16) 4_565 . ?
N11 Cs6A N13 143.77(19) 4_565 . ?
N14 Cs6A N13 77.64(16) . . ?
O3 Cs6A N13 141.5(4) 4_565 . ?
N24 Cs6A C41 74.5(2) . 2_655 ?
N22 Cs6A C41 135.2(2) 4_565 2_655 ?
N11 Cs6A C41 97.28(19) 4_565 2_655 ?
N14 Cs6A C41 149.3(2) . 2_655 ?
O3 Cs6A C41 109.3(4) 4_565 2_655 ?
N13 Cs6A C41 101.3(2) . 2_655 ?
N24 Cs6A C14 70.02(14) . . ?
N22 Cs6A C14 70.52(13) 4_565 . ?
N11 Cs6A C14 116.30(17) 4_565 . ?
N14 Cs6A C14 17.88(13) . . ?
O3 Cs6A C14 81.7(4) 4_565 . ?
N13 Cs6A C14 59.91(15) . . ?
C41 Cs6A C14 143.4(2) 2_655 . ?
N24 Cs6A C11 156.86(18) . 4_565 ?
N22 Cs6A C11 68.01(13) 4_565 4_565 ?
N11 Cs6A C11 17.70(14) 4_565 4_565 ?
```

```
N14 Cs6A C11 111.47(16) . 4_565 ?
O3 Cs6A C11 72.1(4) 4_565 4_565 ?
N13 Cs6A C11 129.70(17) . 4_565 ?
C41 Cs6A C11 92.98(19) 2_655 4_565 ?
C14 Cs6A C11 123.40(15) . 4_565 ?
N24 Cs6A C42 72.1(2) . 2_655 ?
N22 Cs6A C42 153.0(2) 4_565 2_655 ?
N11 Cs6A C42 76.5(2) 4_565 2_655 ?
N14 Cs6A C42 115.8(2) . 2_655 ?
O3 Cs6A C42 64.0(3) 4_565 2_655 ?
N13 Cs6A C42 137.3(2) . 2_655 ?
C41 Cs6A C42 45.8(2) 2_655 2_655 ?
C14 Cs6A C42 126.2(2) . 2_655 ?
C11 Cs6A C42 85.2(2) 4_565 2_655 ?
N24 Cs6A N12 129.64(16) . 4_565 ?
N22 Cs6A N12 66.67(14) 4_565 4_565 ?
N11 Cs6A N12 76.21(15) 4_565 4_565 ?
N14 Cs6A N12 139.74(18) . 4_565 ?
O3 Cs6A N12 130.4(4) 4_565 4_565 ?
N13 Cs6A N12 82.00(16) . 4_565 ?
C41 Cs6A N12 68.7(2) 2_655 4_565 ?
C14 Cs6A N12 130.77(17) . 4_565 ?
C11 Cs6A N12 58.86(14) 4_565 4_565 ?
C42 Cs6A N12 102.8(2) 2_655 4_565 ?
N24 Cs6A C24 15.52(12) . . ?
N22 Cs6A C24 119.05(15) 4_565 . ?
N11 Cs6A C24 149.72(18) 4_565 . ?
N14 Cs6A C24 63.76(13) . . ?
O3 Cs6A C24 95.6(3) 4_565 . ?
N13 Cs6A C24 62.10(14) . . ?
C41 Cs6A C24 88.3(2) 2_655 . ?
C14 Cs6A C24 55.43(12) . . ?
C11 Cs6A C24 167.33(17) 4_565 . ?
C42 Cs6A C24 86.7(2) 2_655 . ?
N12 Cs6A C24 132.78(15) 4_565 . ?

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              30.51
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    2.822
_refine_diff_density_min   -4.528
_refine_diff_density_rms    0.228
```