Unsymmetrical Zirconacyclopentadienes from Isolated Zirconacyclopropenes with 1-Alkynylphosphine Ligands

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Contribution from the Department of Chemistry, University of California, Berkeley, Berkeley, California 94720-1460

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Gaussian03 Output for the Calculation of the Radius of Compound 1:

```
Entering Gaussian System, Link 0=/usr/software/gaussian/g03.revD01/g03
 Initial command:
 /usr/software/gaussian/g03.revD01/l1.exe /scr/77338.bedrock.Felix/Gau-
28698.inp -scrdir=/scr/77338.bedrock.Felix/
 Entering Link 1 = /usr/software/gaussian/g03.revD01/l1.exe PID=
28700.

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Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

*****************************************
Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               30-Apr-2008
*****************************************
%chk=dimer1.chk
%mem=1GB
%nproc=1
Will use up to    1 processors via shared memory.
-----------------------------------------------
# volume=tight b3lyp/lanl2dz geom=connectivity
-----------------------------------------------
1/38=1,57=2/1;
2/17=6,18=5,40=1/2;
3/5=6,6=3,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,32=1,38=5/2;
6/7=2,8=2,9=2,10=2,28=1,44=1,45=100/1,4;
99/5=1,9=1/99;
-----------
volume calc
-----------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
Zr
P                     1    B1
C                     1    B2       2    A1
H                     3    B3       1    A2       2    D1       0
C                     3    B4       1    A3       2    D2       0
H                     5    B5       3    A4       1    D3       0
C                     5    B6       3    A5       1    D4       0
H                     7    B7       5    A6       3    D5       0
C                     7    B8       5    A7       3    D6       0
H                     9    B9       7    A8       5    D7       0
C                     3    B10      1    A9       5    D8       0
```

H	11	B11	3	A10	1	D9	0
C	1	B12	3	A11	11	D10	0
H	13	B13	1	A12	3	D11	0
C	13	B14	1	A13	3	D12	0
H	15	B15	13	A14	1	D13	0
C	15	B16	13	A15	1	D14	0
H	17	B17	15	A16	13	D15	0
C	17	B18	15	A17	13	D16	0
H	19	B19	17	A18	15	D17	0
C	13	B20	1	A19	19	D18	0
H	21	B21	13	A20	1	D19	0
C	2	B22	1	A21	19	D20	0
C	23	B23	2	A22	1	D21	0
C	24	B24	23	A23	2	D22	0
C	25	B25	24	A24	23	D23	0
H	26	B26	25	A25	24	D24	0
C	26	B27	25	A26	24	D25	0
H	28	B28	26	A27	25	D26	0
C	28	B29	26	A28	25	D27	0
H	30	B30	28	A29	26	D28	0
C	30	B31	28	A30	26	D29	0
H	32	B32	30	A31	28	D30	0
C	32	B33	30	A32	28	D31	0
H	34	B34	32	A33	30	D32	0
C	2	B35	1	A34	19	D33	0
H	36	B36	2	A35	1	D34	0
C	36	B37	2	A36	1	D35	0
H	38	B38	36	A37	2	D36	0
H	38	B39	36	A38	2	D37	0
H	38	B40	36	A39	2	D38	0
C	36	B41	2	A40	1	D39	0
H	42	B42	36	A41	2	D40	0
H	42	B43	36	A42	2	D41	0
H	42	B44	36	A43	2	D42	0
C	2	B45	1	A44	19	D43	0
H	46	B46	2	A45	1	D44	0
C	46	B47	2	A46	1	D45	0
H	48	B48	46	A47	2	D46	0
H	48	B49	46	A48	2	D47	0
H	48	B50	46	A49	2	D48	0
C	46	B51	2	A50	1	D49	0
H	52	B52	46	A51	2	D50	0
H	52	B53	46	A52	2	D51	0
H	52	B54	46	A53	2	D52	0
Zr	24	B55	23	A54	2	D53	0
P	56	B56	24	A55	23	D54	0
C	56	B57	24	A56	23	D55	0
H	58	B58	56	A57	24	D56	0
C	58	B59	56	A58	24	D57	0
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H	64	B64	62	A63	60	D62	0
C	58	B65	56	A64	24	D63	0
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C	70	B71	68	A70	56	D69	0
H	72	B72	70	A71	68	D70	0
C	72	B73	70	A72	68	D71	0
H	74	B74	72	A73	70	D72	0
C	68	B75	56	A74	24	D73	0
H	76	B76	68	A75	56	D74	0
C	57	B77	56	A76	24	D75	0
C	78	B78	57	A77	56	D76	0
C	79	B79	78	A78	57	D77	0
C	80	B80	79	A79	78	D78	0
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C	81	B82	80	A81	79	D80	0
H	83	B83	81	A82	80	D81	0
C	83	B84	81	A83	80	D82	0
H	85	B85	83	A84	81	D83	0
C	85	B86	83	A85	81	D84	0
H	87	B87	85	A86	83	D85	0
C	87	B88	85	A87	83	D86	0
H	89	B89	87	A88	85	D87	0
C	57	B90	56	A89	24	D88	0
H	91	B91	57	A90	56	D89	0
C	91	B92	57	A91	56	D90	0
H	93	B93	91	A92	57	D91	0
H	93	B94	91	A93	57	D92	0
H	93	B95	91	A94	57	D93	0
C	91	B96	57	A95	56	D94	0
H	97	B97	91	A96	57	D95	0
H	97	B98	91	A97	57	D96	0
H	97	B99	91	A98	57	D97	0
C	57	B100	56	A99	24	D98	0
H	101	B101	57	A100	56	D99	0
C	101	B102	57	A101	56	D100	0
H	103	B103	101	A102	57	D101	0
H	103	B104	101	A103	57	D102	0
H	103	B105	101	A104	57	D103	0
C	101	B106	57	A105	56	D104	0
H	107	B107	101	A106	57	D105	0
H	107	B108	101	A107	57	D106	0
H	107	B109	101	A108	57	D107	0

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B7	0.98073
B8	1.40751
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B10	1.38958
B11	0.97936
B12	2.59092
B13	0.98034
B14	1.37794

B15	0.97953
B16	1.38653
B17	0.98098
B18	1.40836
B19	0.98106
B20	1.39842
B21	0.98002
B22	1.80602
B23	1.30649
B24	1.47021
B25	1.39356
B26	0.92994
B27	1.38731
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B33	1.38763
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B37	1.52209
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B39	0.95932
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B56	2.79804
B57	2.53336
B58	0.98017
B59	1.40229
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B61	1.38751
B62	0.98083
B63	1.40744
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B65	1.38958
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B69	1.37801
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B77	1.80611
B78	1.30654
B79	1.47021
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B88	1.38763
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B95	0.95996
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B99	0.95997
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B104	0.95967
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B107	0.96087
B108	0.95996
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A1	138.34229
A2	125.45853
A3	74.11848
A4	125.62793
A5	108.10417
A6	125.40219
A7	108.17514
A8	126.07583
A9	76.54717
A10	125.5774
A11	93.13533
A12	125.97319
A13	73.47948
A14	125.08358
A15	109.29909
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A20	125.35792
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A38	109.42121
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A65	125.57186
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A67	125.97618
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A69	125.07847
A70	109.30635
A71	125.42981
A72	108.24496
A73	126.2463
A74	71.61237
A75	125.35867
A76	106.8512

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A98	109.48847
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A107	109.44643
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D9	-121.39707
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D16	-0.20682
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D19	124.0812
D20	-46.0805
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D22	6.22527
D23	-71.10003
D24	1.8899
D25	-178.12251

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D37	59.67903
D38	-60.41591
D39	149.69111
D40	-179.55596
D41	60.38673
D42	-59.65722
D43	72.9853
D44	-68.81521
D45	175.31867
D46	179.52039
D47	59.47013
D48	-60.51814
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D51	60.25597
D52	-59.7432
D53	-170.51461
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D55	-130.5738
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D73	18.08885
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D76	112.38853
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D82	0.06693

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D89	33.85076
D90	-81.12736
D91	179.64956
D92	59.68572
D93	-60.41376
D94	149.69254
D95	-179.55629
D96	60.38843
D97	-59.66086
D98	155.77271
D99	-68.80677
D100	175.31968
D101	179.52269
D102	59.47167
D103	-60.50996
D104	45.36823
D105	-179.7355
D106	60.25649
D107	-59.74134

Stoichiometry C48H58P2Zr2
Framework group C1[X(C48H58P2Zr2)]
Deg. of freedom 324
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	40	0	-1.795361	1.855180	-0.196600
2	15	0	0.738865	1.828002	0.989300
3	6	0	-4.137364	2.644477	0.360301
4	1	0	-4.936099	2.484066	-0.184699
5	6	0	-3.343396	3.799627	0.316305
6	1	0	-3.495687	4.575661	-0.263393
7	6	0	-2.444190	3.745216	1.371605
8	1	0	-1.855150	4.476578	1.654407
9	6	0	-2.707796	2.578390	2.113301
10	1	0	-2.319402	2.347272	2.983201
11	6	0	-3.766692	1.914499	1.483099
12	1	0	-4.239385	1.132771	1.836097
13	6	0	-1.504543	3.599380	-2.090296
14	1	0	-1.679741	4.561304	-2.019093
15	6	0	-0.280892	2.986157	-1.931097
16	1	0	0.558547	3.448638	-1.728796
17	6	0	-0.389168	1.649220	-2.282301
18	1	0	0.362263	1.030097	-2.402102
19	6	0	-1.719833	1.402020	-2.671802
20	1	0	-2.051545	0.597674	-3.125104

21	6	0	-2.413699	2.628079	-2.521098
22	1	0	-3.325001	2.804108	-2.835698
23	6	0	1.592949	0.363889	0.365896
24	6	0	2.625876	0.190617	-0.415104
25	6	0	3.688548	0.931062	-1.110802
26	6	0	3.441413	1.740824	-2.217700
27	1	0	2.567580	1.842338	-2.519200
28	6	0	4.467810	2.398766	-2.879698
29	1	0	4.275494	2.931938	-3.616697
30	6	0	5.779321	2.263059	-2.450799
31	1	0	6.467431	2.711443	-2.886297
32	6	0	6.043357	1.459807	-1.377701
33	1	0	6.920574	1.358590	-1.086501
34	6	0	5.023040	0.792800	-0.714703
35	1	0	5.229938	0.242672	0.007296
36	6	0	0.680632	1.625567	2.853999
37	1	0	-0.091079	1.046214	3.029098
38	6	0	0.392740	2.920525	3.600303
39	1	0	0.370903	2.748645	4.544202
40	1	0	-0.455894	3.268679	3.319403
41	1	0	1.082473	3.560174	3.408404
42	6	0	1.880227	0.904211	3.471097
43	1	0	1.760949	0.841111	4.421597
44	1	0	2.682831	1.395014	3.280999
45	1	0	1.949418	0.021795	3.099295
46	6	0	1.902219	3.253810	0.673104
47	1	0	2.149934	3.175928	-0.271797
48	6	0	3.234687	3.235152	1.440004
49	1	0	3.754675	4.004329	1.198406
50	1	0	3.720716	2.437851	1.218102
51	1	0	3.059813	3.251328	2.383904
52	6	0	1.224664	4.617942	0.798507
53	1	0	1.865323	5.311965	0.622509
54	1	0	0.876812	4.721522	1.687208
55	1	0	0.506639	4.677628	0.164607
56	40	0	1.795366	-1.855132	-0.196610
57	15	0	-0.738785	-1.828028	0.989290
58	6	0	4.137303	-2.644506	0.360288
59	1	0	4.936038	-2.484092	-0.184711
60	6	0	3.343401	-3.799582	0.316285
61	1	0	3.495767	-4.575680	-0.263417
62	6	0	2.444196	-3.745177	1.371585
63	1	0	1.855088	-4.476614	1.654383
64	6	0	2.707734	-2.578428	2.113288
65	1	0	2.319339	-2.347315	2.983189
66	6	0	3.766630	-1.914534	1.483090
67	1	0	4.239464	-1.132801	1.836092
68	6	0	1.504556	-3.599463	-2.090315
69	1	0	1.679680	-4.561320	-2.019117
70	6	0	0.280898	-2.986099	-1.931113
71	1	0	-0.558541	-3.448581	-1.728815
72	6	0	0.389107	-1.649235	-2.282310
73	1	0	-0.362324	-1.030112	-2.402108
74	6	0	1.719839	-1.401958	-2.671809
75	1	0	2.051625	-0.597678	-3.125107
76	6	0	2.413638	-2.628093	-2.521112
77	1	0	3.325008	-2.804045	-2.835712

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   78          6             0       -1.592943   -0.363844    0.365894
   79          6             0       -2.625937   -0.190642   -0.415106
   80          6             0       -3.688609   -0.931083   -1.110808
   81          6             0       -3.441333   -1.740833   -2.217710
   82          1             0       -2.567573   -1.842277   -2.519211
   83          6             0       -4.467870   -2.398777   -2.879712
   84          1             0       -4.275413   -2.931940   -3.616714
   85          6             0       -5.779314   -2.262999   -2.450812
   86          1             0       -6.467492   -2.711455   -2.886313
   87          6             0       -6.043277   -1.459820   -1.377710
   88          1             0       -6.920494   -1.358605   -1.086510
   89          6             0       -5.022960   -0.792817   -0.714708
   90          1             0       -5.229999   -0.242699    0.007293
   91          6             0       -0.680552   -1.625603    2.853990
   92          1             0        0.091017   -1.046257    3.029092
   93          6             0       -0.392728   -2.920639    3.600287
   94          1             0       -0.370966   -2.748696    4.544187
   95          1             0        0.455899   -3.268650    3.319386
   96          1             0       -1.082394   -3.560213    3.408385
   97          6             0       -1.880289   -0.904256    3.471092
   98          1             0       -1.761012   -0.841162    4.421592
   99          1             0       -2.682820   -1.395126    3.280991
  100          1             0       -1.949406   -0.021906    3.099294
  101          6             0       -1.902214   -3.253767    0.673086
  102          1             0       -2.149922   -3.176021   -0.271814
  103          6             0       -3.234749   -3.235187    1.439986
  104          1             0       -3.754737   -4.004363    1.198384
  105          1             0       -3.720704   -2.437952    1.218088
  106          1             0       -3.059807   -3.251294    2.383886
  107          6             0       -1.224659   -4.617899    0.798482
  108          1             0       -1.865385   -5.311996    0.622480
  109          1             0       -0.876806   -4.721484    1.687182
  110          1             0       -0.506559   -4.677649    0.164582
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.0657170      0.0526710
0.0425838
 Standard basis: LANL2DZ (5D, 7F)
 There are   608 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   608 basis functions,  1556 primitive gaussians,   612 cartesian
basis functions
   190 alpha electrons      190 beta electrons
       nuclear repulsion energy      7822.4969087571 Hartrees.


 Warning!  P  atom    2 may be hypervalent but has no d functions.
 Warning!  P  atom   57 may be hypervalent but has no d functions.


 NAtoms=  110 NActive=  110 NUniq=  110 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=T Big=T
 One-electron integrals computed using PRISM.
   1 Symmetry operations used in ECPInt.
```

```
 ECPInt:  NShTT=   72390 NPrTT=  502054 LenC2=   62705 LenP2D=  223428.
 LDataN:  DoStor=F MaxTD1= 5 Len=  102
 LDataN:  DoStor=T MaxTD1= 5 Len=  102
 NBasis=   608 RedAO= T  NBF=   608
 NBsUse=   608 1.00D-06 NBFU=   608
 Defaulting to unpruned grid for atomic number  40.
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 2.43D-02 ExpMax= 4.23D+03 ExpMxC= 1.46D+02 IAcc=3 IRadAn=
5 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Defaulting to unpruned grid for atomic number  40.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-04 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-02.
 Requested convergence on             energy=1.00D-02.
 No special actions if energy rises.
 Defaulting to unpruned grid for atomic number  40.
 SCF Done:  E(RB+HF-LYP) =  -1969.06207600     A.U. after    8 cycles
             Convg  =    0.6546D-04             -V/T =  2.0357
             S**2   =   0.0000

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            Population analysis using the SCF density.

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 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -10.19081 -10.19080 -10.17447 -10.17446 -
10.17104
 Alpha  occ. eigenvalues --  -10.17104 -10.17091 -10.17091 -10.17042 -
10.17042
 Alpha  occ. eigenvalues --  -10.17035 -10.17035 -10.16989 -10.16988 -
10.16968
 Alpha  occ. eigenvalues --  -10.16967 -10.16953 -10.16953 -10.16914 -
10.16913
 Alpha  occ. eigenvalues --  -10.16902 -10.16901 -10.16749 -10.16749 -
10.16691
 Alpha  occ. eigenvalues --  -10.16690 -10.16489 -10.16489 -10.16191 -
10.16191
 Alpha  occ. eigenvalues --  -10.16105 -10.16105 -10.16097 -10.16097 -
10.16036
 Alpha  occ. eigenvalues --  -10.16035 -10.15247 -10.15246 -10.14263 -
10.14263
 Alpha  occ. eigenvalues --  -10.13794 -10.13793 -10.13220 -10.13219 -
10.13096
 Alpha  occ. eigenvalues --  -10.13095 -10.12708 -10.12707  -1.98706  -
1.98706
 Alpha  occ. eigenvalues --   -1.20014  -1.20012  -1.18681  -1.18674  -
1.17891
 Alpha  occ. eigenvalues --   -1.17889  -0.89220  -0.89180  -0.88373  -
0.88334
 Alpha  occ. eigenvalues --   -0.85742  -0.85740  -0.82959  -0.82606  -
0.80535
 Alpha  occ. eigenvalues --   -0.80315  -0.77335  -0.77305  -0.75528  -
0.75528
 Alpha  occ. eigenvalues --   -0.73194  -0.73192  -0.72418  -0.72342  -
0.72323
 Alpha  occ. eigenvalues --   -0.72123  -0.72119  -0.71995  -0.71938  -
0.71806
 Alpha  occ. eigenvalues --   -0.71717  -0.71691  -0.71541  -0.71230  -
0.66440
 Alpha  occ. eigenvalues --   -0.66376  -0.62615  -0.62605  -0.61785  -
0.61663
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 Alpha  occ. eigenvalues --   -0.61524  -0.61288  -0.56925  -0.56681  -
0.56496
 Alpha  occ. eigenvalues --   -0.56175  -0.56167  -0.55920  -0.55890  -
0.55801
 Alpha  occ. eigenvalues --   -0.55592  -0.55494  -0.55421  -0.55313  -
0.55185
 Alpha  occ. eigenvalues --   -0.54516  -0.54476  -0.54199  -0.50703  -
0.50389
 Alpha  occ. eigenvalues --   -0.48970  -0.48516  -0.47034  -0.46503  -
0.46104
 Alpha  occ. eigenvalues --   -0.45951  -0.45740  -0.45521  -0.44631  -
0.44630
 Alpha  occ. eigenvalues --   -0.44099  -0.44098  -0.43500  -0.43288  -
0.43055
 Alpha  occ. eigenvalues --   -0.43049  -0.42897  -0.42895  -0.42597  -
0.42589
 Alpha  occ. eigenvalues --   -0.41744  -0.41251  -0.41115  -0.41046  -
0.40804
 Alpha  occ. eigenvalues --   -0.40792  -0.40745  -0.40588  -0.40505  -
0.40358
 Alpha  occ. eigenvalues --   -0.40317  -0.39905  -0.38676  -0.38479  -
0.38454
 Alpha  occ. eigenvalues --   -0.38423  -0.38116  -0.38095  -0.38071  -
0.37887
 Alpha  occ. eigenvalues --   -0.37814  -0.37485  -0.37123  -0.37086  -
0.36492
 Alpha  occ. eigenvalues --   -0.36371  -0.36184  -0.36131  -0.35822  -
0.35752
 Alpha  occ. eigenvalues --   -0.35341  -0.35234  -0.34940  -0.34910  -
0.34396
 Alpha  occ. eigenvalues --   -0.34210  -0.34050  -0.33822  -0.31666  -
0.30774
 Alpha  occ. eigenvalues --   -0.30368  -0.29562  -0.27482  -0.27168  -
0.25907
 Alpha  occ. eigenvalues --   -0.25813  -0.25582  -0.25111  -0.24447  -
0.24420
 Alpha  occ. eigenvalues --   -0.23900  -0.23683  -0.23537  -0.23329  -
0.21684
 Alpha  occ. eigenvalues --   -0.21517  -0.20084  -0.19855  -0.17445  -
0.16765
 Alpha virt. eigenvalues --   -0.01525  -0.00333  -0.00204  -0.00075
0.00145
 Alpha virt. eigenvalues --    0.00648   0.00752   0.00858   0.01807
0.02375
 Alpha virt. eigenvalues --    0.02766   0.02917   0.03134   0.03573
0.03788
 Alpha virt. eigenvalues --    0.03980   0.04195   0.04211   0.05311
0.05347
 Alpha virt. eigenvalues --    0.05878   0.06442   0.07046   0.07414
0.08002
 Alpha virt. eigenvalues --    0.08336   0.08382   0.08500   0.08591
0.09785
 Alpha virt. eigenvalues --    0.10388   0.10671   0.11476   0.11680
0.11889
 Alpha virt. eigenvalues --    0.12001   0.12048   0.12584   0.13463
0.13953
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 Alpha virt. eigenvalues --    0.14011   0.14310   0.14571   0.15019
0.15126
 Alpha virt. eigenvalues --    0.15320   0.15624   0.15754   0.16018
0.16270
 Alpha virt. eigenvalues --    0.16409   0.16667   0.16877   0.17039
0.17250
 Alpha virt. eigenvalues --    0.17306   0.17595   0.17667   0.17767
0.18129
 Alpha virt. eigenvalues --    0.18273   0.18556   0.18816   0.18879
0.19261
 Alpha virt. eigenvalues --    0.19815   0.19891   0.19964   0.19991
0.20520
 Alpha virt. eigenvalues --    0.20728   0.20809   0.20840   0.21507
0.21641
 Alpha virt. eigenvalues --    0.22000   0.22284   0.22363   0.22614
0.22726
 Alpha virt. eigenvalues --    0.22936   0.23275   0.23752   0.24149
0.24301
 Alpha virt. eigenvalues --    0.24478   0.24771   0.24906   0.25136
0.25365
 Alpha virt. eigenvalues --    0.25772   0.25915   0.26378   0.26611
0.26740
 Alpha virt. eigenvalues --    0.27046   0.27064   0.27234   0.27382
0.27662
 Alpha virt. eigenvalues --    0.27750   0.28247   0.28375   0.28611
0.28907
 Alpha virt. eigenvalues --    0.29314   0.29674   0.29767   0.30174
0.30303
 Alpha virt. eigenvalues --    0.30421   0.30684   0.30969   0.30988
0.31474
 Alpha virt. eigenvalues --    0.31476   0.31736   0.31976   0.32151
0.32508
 Alpha virt. eigenvalues --    0.32570   0.32931   0.33100   0.33114
0.33440
 Alpha virt. eigenvalues --    0.33605   0.33688   0.33761   0.33925
0.34012
 Alpha virt. eigenvalues --    0.34113   0.34714   0.34752   0.34864
0.35316
 Alpha virt. eigenvalues --    0.35597   0.35613   0.35665   0.36350
0.36579
 Alpha virt. eigenvalues --    0.36682   0.37124   0.37142   0.37487
0.37633
 Alpha virt. eigenvalues --    0.37703   0.37816   0.38052   0.38067
0.38740
 Alpha virt. eigenvalues --    0.38856   0.38890   0.39190   0.39278
0.39810
 Alpha virt. eigenvalues --    0.39819   0.40109   0.40570   0.40633
0.40830
 Alpha virt. eigenvalues --    0.41042   0.41239   0.41264   0.41649
0.41788
 Alpha virt. eigenvalues --    0.41876   0.42140   0.42411   0.42413
0.42461
 Alpha virt. eigenvalues --    0.42588   0.42923   0.43237   0.43476
0.43561
 Alpha virt. eigenvalues --    0.43840   0.44241   0.44452   0.44487
0.44706
```

```
 Alpha virt. eigenvalues --    0.44785   0.44975   0.45225   0.45722
0.45906
 Alpha virt. eigenvalues --    0.45943   0.46261   0.46507   0.46913
0.47676
 Alpha virt. eigenvalues --    0.47833   0.48267   0.48832   0.49020
0.49077
 Alpha virt. eigenvalues --    0.49409   0.49684   0.50058   0.50246
0.50592
 Alpha virt. eigenvalues --    0.50760   0.51349   0.51520   0.51579
0.51985
 Alpha virt. eigenvalues --    0.52114   0.52412   0.52682   0.53290
0.53487
 Alpha virt. eigenvalues --    0.53698   0.53861   0.54233   0.54694
0.55066
 Alpha virt. eigenvalues --    0.55785   0.55894   0.55999   0.56530
0.56860
 Alpha virt. eigenvalues --    0.57118   0.57195   0.58222   0.58464
0.59104
 Alpha virt. eigenvalues --    0.59516   0.60038   0.60127   0.60146
0.60308
 Alpha virt. eigenvalues --    0.61079   0.61178   0.62113   0.62640
0.62963
 Alpha virt. eigenvalues --    0.63023   0.63433   0.64414   0.64897
0.65011
 Alpha virt. eigenvalues --    0.65309   0.65310   0.65797   0.66001
0.66166
 Alpha virt. eigenvalues --    0.66486   0.67165   0.67525   0.68066
0.68825
 Alpha virt. eigenvalues --    0.69063   0.69206   0.69494   0.69999
0.70241
 Alpha virt. eigenvalues --    0.70988   0.71007   0.71345   0.71514
0.72293
 Alpha virt. eigenvalues --    0.72639   0.73342   0.73465   0.73785
0.74172
 Alpha virt. eigenvalues --    0.74561   0.75311   0.75378   0.75962
0.75978
 Alpha virt. eigenvalues --    0.76142   0.76243   0.76519   0.76662
0.76874
 Alpha virt. eigenvalues --    0.77307   0.77339   0.77971   0.78757
0.78988
 Alpha virt. eigenvalues --    0.79370   0.79762   0.80544   0.80586
0.81232
 Alpha virt. eigenvalues --    0.81606   0.81791   0.83164   0.83475
0.83733
 Alpha virt. eigenvalues --    0.84323   0.85893   0.85904   0.87228
0.88978
 Alpha virt. eigenvalues --    0.89533   0.89801   0.90194   0.91681
0.93032
 Alpha virt. eigenvalues --    0.93854   0.95121   0.96580   0.98792
1.01288
 Alpha virt. eigenvalues --    1.03344   1.04484   1.04835   1.06205
1.10538
 Alpha virt. eigenvalues --    1.10658   1.12841   1.13150   1.14192
1.15302
 Alpha virt. eigenvalues --    1.15947   1.16705   1.18229   1.18579
1.19039
```

```
 Alpha virt. eigenvalues --    1.19254   1.19978   1.20430   1.21380
1.22684
 Alpha virt. eigenvalues --    1.23015   1.23334   1.24056   1.25954
1.26430
 Alpha virt. eigenvalues --    1.27628   1.27762   1.28379   1.28771
1.29285
 Alpha virt. eigenvalues --    1.29833   1.29895   1.30829   1.31386
1.31701
 Alpha virt. eigenvalues --    1.31721   1.32594   1.32761   1.33309
1.34057
 Alpha virt. eigenvalues --    1.34791   1.35188   1.35641   1.35796
1.36419
 Alpha virt. eigenvalues --    1.37144   1.37241   1.37254   1.38773
1.38922
 Alpha virt. eigenvalues --    1.39836   1.39925   1.40374   1.40839
1.41060
 Alpha virt. eigenvalues --    1.41801   1.42610   1.43312   1.43353
1.44037
 Alpha virt. eigenvalues --    1.44493   1.44559   1.45534   1.45973
1.46056
 Alpha virt. eigenvalues --    1.46361   1.47255   1.47643   1.47802
1.48771
 Alpha virt. eigenvalues --    1.49020   1.49356   1.50492   1.50910
1.51965
 Alpha virt. eigenvalues --    1.52507   1.53465   1.54246   1.54897
1.55258
 Alpha virt. eigenvalues --    1.55511   1.55738   1.56172   1.57322
1.57412
 Alpha virt. eigenvalues --    1.58416   1.58886   1.59916   1.60130
1.61212
 Alpha virt. eigenvalues --    1.61927   1.62084   1.62529   1.62574
1.64770
 Alpha virt. eigenvalues --    1.65492   1.65755   1.66875   1.67658
1.67778
 Alpha virt. eigenvalues --    1.68027   1.70454   1.71758   1.71915
1.72003
 Alpha virt. eigenvalues --    1.74850   1.77678   1.79808   1.83111
15.23445
 Alpha virt. eigenvalues --   16.12754  19.41834  19.77172
          Condensed to atoms (all electrons):
 Mulliken atomic charges:
              1
     1  Zr   0.805204
     2  P    0.569686
     3  C   -0.336429
     4  H    0.321903
     5  C   -0.372480
     6  H    0.329777
     7  C   -0.350507
     8  H    0.319373
     9  C   -0.351755
    10  H    0.311778
    11  C   -0.333927
    12  H    0.320417
    13  C   -0.356588
    14  H    0.325786
    15  C   -0.359653
```

16	H	0.331129
17	C	-0.294337
18	H	0.327495
19	C	-0.376646
20	H	0.344142
21	C	-0.377596
22	H	0.324972
23	C	-0.445341
24	C	-0.288654
25	C	0.340558
26	C	-0.563147
27	H	0.352350
28	C	-0.326674
29	H	0.312001
30	C	-0.340273
31	H	0.312844
32	C	-0.317517
33	H	0.305469
34	C	-0.537226
35	H	0.334981
36	C	-0.427864
37	H	0.287404
38	C	-0.774995
39	H	0.242229
40	H	0.274512
41	H	0.246147
42	C	-0.763749
43	H	0.232567
44	H	0.270034
45	H	0.285231
46	C	-0.440482
47	H	0.290258
48	C	-0.751348
49	H	0.236573
50	H	0.287274
51	H	0.232490
52	C	-0.763540
53	H	0.244020
54	H	0.261419
55	H	0.270677
56	Zr	0.805228
57	P	0.569643
58	C	-0.336438
59	H	0.321922
60	C	-0.372419
61	H	0.329722
62	C	-0.350425
63	H	0.319303
64	C	-0.351750
65	H	0.311790
66	C	-0.333905
67	H	0.320344
68	C	-0.356676
69	H	0.325849
70	C	-0.359620
71	H	0.331124
72	C	-0.294323

```
    73  H    0.327490
    74  C   -0.376712
    75  H    0.344174
    76  C   -0.377521
    77  H    0.324935
    78  C   -0.445303
    79  C   -0.288713
    80  C    0.340718
    81  C   -0.563305
    82  H    0.352453
    83  C   -0.326635
    84  H    0.311977
    85  C   -0.340192
    86  H    0.312771
    87  C   -0.317511
    88  H    0.305471
    89  C   -0.537279
    90  H    0.334968
    91  C   -0.427982
    92  H    0.287484
    93  C   -0.775002
    94  H    0.242211
    95  H    0.274527
    96  H    0.246195
    97  C   -0.763754
    98  H    0.232560
    99  H    0.270041
   100  H    0.285261
   101  C   -0.440492
   102  H    0.290267
   103  C   -0.751356
   104  H    0.236568
   105  H    0.287317
   106  H    0.232474
   107  C   -0.763514
   108  H    0.243981
   109  H    0.261430
   110  H    0.270657
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
     1  Zr   0.805204
     2  P    0.569686
     3  C   -0.014526
     4  H    0.000000
     5  C   -0.042703
     6  H    0.000000
     7  C   -0.031134
     8  H    0.000000
     9  C   -0.039977
    10  H    0.000000
    11  C   -0.013510
    12  H    0.000000
    13  C   -0.030801
    14  H    0.000000
    15  C   -0.028524
    16  H    0.000000
```

17	C	0.033158
18	H	0.000000
19	C	-0.032504
20	H	0.000000
21	C	-0.052624
22	H	0.000000
23	C	-0.445341
24	C	-0.288654
25	C	0.340558
26	C	-0.210797
27	H	0.000000
28	C	-0.014673
29	H	0.000000
30	C	-0.027428
31	H	0.000000
32	C	-0.012048
33	H	0.000000
34	C	-0.202244
35	H	0.000000
36	C	-0.140460
37	H	0.000000
38	C	-0.012106
39	H	0.000000
40	H	0.000000
41	H	0.000000
42	C	0.024082
43	H	0.000000
44	H	0.000000
45	H	0.000000
46	C	-0.150224
47	H	0.000000
48	C	0.004989
49	H	0.000000
50	H	0.000000
51	H	0.000000
52	C	0.012575
53	H	0.000000
54	H	0.000000
55	H	0.000000
56	Zr	0.805228
57	P	0.569643
58	C	-0.014516
59	H	0.000000
60	C	-0.042696
61	H	0.000000
62	C	-0.031123
63	H	0.000000
64	C	-0.039959
65	H	0.000000
66	C	-0.013561
67	H	0.000000
68	C	-0.030826
69	H	0.000000
70	C	-0.028496
71	H	0.000000
72	C	0.033167
73	H	0.000000

```
   74  C   -0.032538
   75  H    0.000000
   76  C   -0.052586
   77  H    0.000000
   78  C   -0.445303
   79  C   -0.288713
   80  C    0.340718
   81  C   -0.210853
   82  H    0.000000
   83  C   -0.014658
   84  H    0.000000
   85  C   -0.027422
   86  H    0.000000
   87  C   -0.012040
   88  H    0.000000
   89  C   -0.202311
   90  H    0.000000
   91  C   -0.140498
   92  H    0.000000
   93  C   -0.012068
   94  H    0.000000
   95  H    0.000000
   96  H    0.000000
   97  C    0.024108
   98  H    0.000000
   99  H    0.000000
  100  H    0.000000
  101  C   -0.150226
  102  H    0.000000
  103  C    0.005003
  104  H    0.000000
  105  H    0.000000
  106  H    0.000000
  107  C    0.012554
  108  H    0.000000
  109  H    0.000000
  110  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>= 27451.7006
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     0.0001    Y=    -0.0001    Z=     2.5738  Tot=     2.5738
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -349.9093   YY=  -337.9545   ZZ=  -350.2965
  XY=     7.7637   XZ=     0.0003   YZ=    -0.0004
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    -3.8558   YY=     8.0989   ZZ=    -4.2431
  XY=     7.7637   XZ=     0.0003   YZ=    -0.0004
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    -0.0038  YYY=     0.0053  ZZZ=    86.0145  XYY=     0.0052
 XXY=    -0.0076  XXZ=   -35.1603  XZZ=     0.0015  YZZ=     0.0045
 YYZ=   -24.4070  XYZ=    15.7773
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=-17277.2895 YYYY=-12834.0108 ZZZZ= -7788.9729 XXXY=   176.6860
XXXZ=    -0.0082 YYYX=   -91.4804 YYYZ=     0.0073 ZZZX=    -0.0171
ZZZY=    -0.0134 XXYY= -5234.2035 XXZZ= -4352.3909 YYZZ= -3505.4169
XXYZ=    -0.0270 YYXZ=     0.0026 ZZXY=   145.4715
```

```
 N-N= 7.822496908757D+03 E-N=-2.018099623087D+04  KE=
1.901100969923D+03
 Evaluate density.
 Using the total density.
 Monte-Carlo method of calculating molar volume:
 based on  0.001 e/bohr**3 density envelope.
 Number of points per bohr**3 =  100 CutOff= 1.00D-04
 Using the SCF density.
 There are      3101 points.  Will hold      3101 in memory.
 LenV=   131934798 MDV=   134217728.
 Box volume =29845.815 fraction occupied=0.212
 Integrated density= 2.871890242756978 1D+02 error=-
9.2810975724302178D+01
 Molar volume = 6332.972 bohr**3/mol (565.148 cm**3/mol)
 Recommended a0 for SCRF calculation =  7.18 angstrom ( 13.58 bohr)
 1\1\GINC-BEDROCK02\SP\RB3LYP\LANL2DZ\C48H58P2Zr2\JAMIN\01-May-2008\0\\
 # volume=tight b3lyp/lanl2dz geom=connectivity\\volume calc\\0,1\Zr\P,
 1,2.79810579\C,1,2.5333988,2,138.34228504\H,3,0.98017103,1,125.4585328
 5,2,-174.26063711,0\C,3,1.40238863,1,74.11848367,2,63.32399787,0\H,5,0
 .98054619,3,125.62792925,1,122.46037577,0\C,5,1.3875117,3,108.10416621
 ,1,-66.87132411,0\H,7,0.98073259,5,125.40219186,3,-171.00950653,0\C,7,
 1.4075104,5,108.17513705,3,-2.30212519,0\H,9,0.98030113,7,126.07583462
 ,5,-170.43928674,0\C,3,1.38958257,1,76.54716759,5,-113.34602502,0\H,11
 ,0.97935998,3,125.57739508,1,-121.39707228,0\C,1,2.59092439,3,93.13532
 788,11,-162.66530458,0\H,13,0.98033744,1,125.97318838,3,50.03849946,0\
 C,13,1.37793704,1,73.47947553,3,172.80727243,0\H,15,0.97952657,13,125.
 08358224,1,-122.93401046,0\C,15,1.38653054,13,109.29908733,1,65.253726
 41,0\H,17,0.98097645,15,125.42730983,13,169.19087853,0\C,17,1.40836318
 ,15,108.24500858,13,-0.20682026,0\H,19,0.98106408,17,126.23888686,15,1
 67.86918032,0\C,13,1.39842023,1,71.61547786,19,37.98457268,0\H,21,0.98
 001611,13,125.35792345,1,124.08119987,0\C,2,1.80602272,1,106.85131726,
 19,-46.08050076,0\C,23,1.30649249,2,133.45193659,1,112.38703798,0\C,24
 ,1.47021289,23,141.95528089,2,6.22527275,0\C,25,1.39356141,24,122.7055
 006,23,-71.10002704,0\H,26,0.92994164,25,119.18245538,24,1.88990019,0\
 C,26,1.38730633,25,121.56041949,24,-178.12250895,0\H,28,0.92974483,26,
 119.81424946,25,179.89467337,0\C,28,1.38651806,26,120.38423616,25,0.06
 562642,0\H,30,0.92962556,28,120.53316256,26,-179.22929728,0\C,30,1.366
 1877,28,118.90313156,26,0.76076984,0\H,32,0.92981293,30,119.49381722,2
 8,179.61072045,0\C,32,1.38762807,30,121.05100557,28,-0.41934857,0\H,34
 ,0.93098333,32,119.41746717,30,179.23171144,0\C,2,1.87655938,1,113.209
 00341,19,-161.99845495,0\H,36,0.98073733,2,105.39979493,1,33.84758835,
 0\C,36,1.52209334,2,113.65988663,1,-81.122511,0\H,38,0.95966983,36,109
 .52286972,2,179.64550403,0\H,38,0.95932031,36,109.42121288,2,59.679034
 59,0\H,38,0.96005553,36,109.44785301,2,-60.41590946,0\C,36,1.5297694,2
 ,115.30124912,1,149.69111008,0\H,42,0.96003053,36,109.44812559,2,-179.
 5559612,0\H,42,0.95979118,36,109.55514405,2,60.3867324,0\H,42,0.960042
 17,36,109.49399232,2,-59.65721725,0\C,2,1.86716447,1,119.01976234,19,7
 2.98530037,0\H,46,0.97993093,2,105.07620007,1,-68.81521186,0\C,46,1.53
 751561,2,116.50216912,1,175.31866948,0\H,48,0.95936953,46,109.5351844,
 2,179.52039328,0\H,48,0.95976811,46,109.48898121,2,59.47012599,0\H,48,
 0.96009897,46,109.40967382,2,-60.51814291,0\C,46,1.52828748,2,113.0463
 5877,1,45.36602728,0\H,52,0.96077448,46,109.51841054,2,-179.73487018,0
 \H,52,0.95995747,46,109.44643063,2,60.25597255,0\H,52,0.95966231,46,10
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 60832,0\P,56,2.79803822,24,111.82841806,23,11.65797164,0\C,56,2.533359
 52,24,87.87454743,23,-130.57379638,0\H,58,0.98017103,56,125.45730502,2
 4,-53.06082812,0\C,58,1.40228962,56,74.12107682,24,-175.47717099,0\H,6
```

0,0.980611,58,125.62668509,56,122.4651292,0\C,60,1.3875117,58,108.1037
3585,56,-66.87127195,0\H,62,0.98082817,60,125.4011464,58,-171.01157982
,0\C,62,1.40743654,60,108.17787151,58,-2.30228314,0\H,64,0.98030113,62
,126.07849306,60,-170.43886646,0\C,58,1.38958257,56,76.5464706,24,71.1
7705503,0\H,66,0.97943335,58,125.57185961,56,-121.40047016,0\C,56,2.59
101877,24,126.21269934,23,137.09893694,0\H,68,0.98025811,56,125.976180
69,24,139.69938825,0\C,68,1.37800568,56,73.47526481,24,-97.53237937,0\
H,70,0.97952657,68,125.07847128,56,-122.9354309,0\C,70,1.38645404,68,1
09.30635462,56,65.25458658,0\H,72,0.98097645,70,125.42981211,68,169.18
969122,0\C,72,1.40843983,70,108.24496477,68,-0.21049899,0\H,74,0.98103
381,72,126.24629986,70,167.86863226,0\C,68,1.39841901,56,71.61236574,2
4,18.08885188,0\H,76,0.98006551,68,125.3586695,56,124.07913136,0\C,57,
1.80611229,56,106.85119879,24,36.70930114,0\C,78,1.30653597,57,133.448
68835,56,112.38853401,0\C,79,1.47021289,78,141.958958,57,6.22361042,0\
C,80,1.3935827,79,122.69978983,78,-71.09691224,0\H,81,0.92986487,80,11
9.18713825,79,1.88485926,0\C,81,1.38741393,80,121.55092943,79,-178.122
0916,0\H,83,0.92977034,81,119.80194691,80,179.89492862,0\C,83,1.386461
55,81,120.38529993,80,0.0669338,0\H,85,0.92971108,83,120.531372,81,-17
9.22522651,0\C,85,1.3661338,83,118.90344067,81,0.75601141,0\H,87,0.929
81293,85,119.4913839,83,179.61303519,0\C,87,1.38762807,85,121.05344017
,83,-0.41404421,0\H,89,0.9310109,87,119.40895138,85,179.22804322,0\C,5
7,1.87655938,56,113.20948577,24,-79.20767194,0\H,91,0.98062234,57,105.
40133746,56,33.85075719,0\C,91,1.52214345,57,113.65864674,56,-81.12735
611,0\H,93,0.95968023,91,109.51687436,57,179.6495576,0\H,93,0.95926331
,91,109.41274909,57,59.68572146,0\H,93,0.95995789,91,109.44997073,57,-
60.4137576,0\C,91,1.52987713,57,115.29913137,56,149.69254039,0\H,97,0.
96003053,91,109.44598699,57,-179.55629003,0\H,97,0.95976386,91,109.553
43381,57,60.38842871,0\H,97,0.95997491,91,109.48847283,57,-59.66086297
,0\C,57,1.86715904,56,119.0231205,24,155.77271175,0\H,101,0.97991807,5
7,105.08349878,56,-68.80676533,0\C,101,1.53757312,57,116.50750467,56,1
75.31967997,0\H,103,0.95936953,101,109.53821042,57,179.52268779,0\H,10
3,0.95967471,101,109.48501244,57,59.47167068,0\H,103,0.96011,101,109.4
0461203,57,-60.50996379,0\C,101,1.52828748,57,113.04333141,56,45.36822
744,0\H,107,0.96087279,101,109.51861435,57,-179.73549539,0\H,107,0.959
95747,101,109.44643063,57,60.25648651,0\H,107,0.95972178,101,109.45712
743,57,-59.74134028,0\\Version=IA32L-G03RevD.01\State=1-A\HF=-1969.062
076\RMSD=6.546e-05\Thermal=0.\Dipole=0.8172547,0.4162342,0.4292014\PG=
C01 [X(C48H58P2Zr2)]\\@

"A LITTLE BIT GOES A LONG WAY"
R.S. MULLIKEN AS QUOTED BY K. RUEDENBERG
Job cpu time: 0 days 6 hours 41 minutes 56.9 seconds.
File lengths (MBytes): RWF=   209 Int=   0 D2E=   0 Chk=
23 Scr=   1
Normal termination of Gaussian 03 at Thu May 1 00:01:52 2008.

Gaussian03 Output for the Calculation of the Radius of Compound 4:

```
Entering Gaussian System, Link 0=/usr/software/gaussian/g03.revD01/g03
 Initial command:
 /usr/software/gaussian/g03.revD01/l1.exe /scr/77339.bedrock.Felix/Gau-
30948.inp -scrdir=/scr/77339.bedrock.Felix/
 Entering Link 1 = /usr/software/gaussian/g03.revD01/l1.exe PID=
30950.

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```

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Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

*****************************************
Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               30-Apr-2008
*****************************************
%chk=monomer1.chk
%mem=1GB
%nproc=1
Will use up to    1 processors via shared memory.
-----------------------------------------------
# volume=tight b3lyp/lanl2dz geom=connectivity
-----------------------------------------------
1/38=1,57=2/1;
2/17=6,18=5,40=1/2;
3/5=6,6=3,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,32=1,38=5/2;
6/7=2,8=2,9=2,10=2,28=1,44=1,45=100/1,4;
99/5=1,9=1/99;
-----------------------
volume calc for monomer
-----------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
Zr
P                     1    B1
N                     1    B2       2    A1
C                     1    B3       3    A2       2    D1       0
C                     4    B4       1    A3       3    D2       0
C                     5    B5       4    A4       1    D3       0
C                     6    B6       5    A5       4    D4       0
C                     7    B7       6    A6       5    D5       0
C                     1    B8       3    A7       6    D6       0
C                     9    B9       1    A8       3    D7       0
C                     10   B10      9    A9       1    D8       0
```

C	11	B11	10	A10	9	D9	0
C	12	B12	11	A11	10	D10	0
C	2	B13	1	A12	3	D11	0
C	14	B14	2	A13	1	D12	0
C	15	B15	14	A14	2	D13	0
C	16	B16	15	A15	14	D14	0
C	17	B17	16	A16	15	D15	0
C	18	B18	17	A17	16	D16	0
C	19	B19	18	A18	17	D17	0
C	20	B20	19	A19	18	D18	0
C	17	B21	16	A20	15	D19	0
C	19	B22	18	A21	17	D20	0
C	21	B23	20	A22	19	D21	0
C	2	B24	1	A23	14	D22	0
C	25	B25	2	A24	1	D23	0
C	26	B26	25	A25	2	D24	0
C	27	B27	26	A26	25	D25	0
C	28	B28	27	A27	26	D26	0
C	25	B29	2	A28	1	D27	0
C	2	B30	1	A29	14	D28	0
C	31	B31	2	A30	1	D29	0
C	32	B32	31	A31	2	D30	0
C	33	B33	32	A32	31	D31	0
C	34	B34	33	A33	32	D32	0
C	35	B35	34	A34	33	D33	0
C	3	B36	1	A35	14	D34	0
C	37	B37	3	A36	1	D35	0
C	38	B38	37	A37	3	D36	0
C	39	B39	38	A38	37	D37	0
C	3	B40	1	A39	14	D38	0
H	4	B41	1	A40	14	D39	0
H	5	B42	4	A41	1	D40	0
H	6	B43	5	A42	4	D41	0
H	7	B44	6	A43	5	D42	0
H	8	B45	7	A44	6	D43	0
H	9	B46	1	A45	14	D44	0
H	10	B47	9	A46	1	D45	0
H	11	B48	10	A47	9	D46	0
H	12	B49	11	A48	10	D47	0
H	13	B50	12	A49	11	D48	0
H	18	B51	17	A50	16	D49	0
H	20	B52	19	A51	18	D50	0
H	22	B53	17	A52	16	D51	0
H	22	B54	17	A53	16	D52	0
H	22	B55	17	A54	16	D53	0
H	23	B56	19	A55	18	D54	0
H	23	B57	19	A56	18	D55	0
H	23	B58	19	A57	18	D56	0
H	24	B59	21	A58	20	D57	0
H	24	B60	21	A59	20	D58	0
H	24	B61	21	A60	20	D59	0
H	26	B62	25	A61	2	D60	0
H	27	B63	26	A62	25	D61	0
H	28	B64	27	A63	26	D62	0
H	29	B65	28	A64	27	D63	0
H	30	B66	25	A65	2	D64	0
H	32	B67	31	A66	2	D65	0

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H                  33   B68      32   A67      31   D66      0
H                  34   B69      33   A68      32   D67      0
H                  35   B70      34   A69      33   D68      0
H                  36   B71      35   A70      34   D69      0
H                  37   B72      3    A71      1    D70      0
H                  38   B73      37   A72      3    D71      0
H                  39   B74      38   A73      37   D72      0
H                  40   B75      39   A74      38   D73      0
H                  41   B76      3    A75      1    D74      0
      Variables:
 B1                    3.75953
 B2                    2.44835
 B3                    2.54146
 B4                    1.40116
 B5                    1.39616
 B6                    1.42151
 B7                    1.39046
 B8                    2.56992
 B9                    1.38506
 B10                   1.40478
 B11                   1.40741
 B12                   1.39203
 B13                   1.78135
 B14                   1.31426
 B15                   1.48209
 B16                   1.40634
 B17                   1.3928
 B18                   1.38429
 B19                   1.38928
 B20                   1.38492
 B21                   1.50147
 B22                   1.51749
 B23                   1.50459
 B24                   1.84113
 B25                   1.39164
 B26                   1.38136
 B27                   1.38244
 B28                   1.37829
 B29                   1.38163
 B30                   1.84443
 B31                   1.39063
 B32                   1.39051
 B33                   1.37417
 B34                   1.39115
 B35                   1.37859
 B36                   1.34257
 B37                   1.38302
 B38                   1.36444
 B39                   1.37967
 B40                   1.33869
 B41                   0.9518
 B42                   0.956
 B43                   0.95137
 B44                   0.95486
 B45                   0.95282
 B46                   0.95112
 B47                   0.95186
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B48	0.94923
B49	0.94826
B50	0.94996
B51	0.95032
B52	0.95452
B53	0.95384
B54	0.96453
B55	0.9515
B56	0.96094
B57	0.95326
B58	0.95082
B59	0.95022
B60	0.95845
B61	0.97193
B62	0.94633
B63	0.94693
B64	0.94776
B65	0.9479
B66	0.94953
B67	0.94994
B68	0.94749
B69	0.94888
B70	0.94972
B71	0.94966
B72	0.95094
B73	0.94921
B74	0.94303
B75	0.94786
B76	0.94678
A1	134.8358
A2	125.94245
A3	75.29932
A4	107.95801
A5	107.84205
A6	107.70359
A7	80.60085
A8	75.16915
A9	108.48734
A10	107.41168
A11	108.18341
A12	21.8268
A13	141.72042
A14	134.75919
A15	120.77357
A16	119.47993
A17	122.24125
A18	117.60536
A19	122.07598
A20	120.50242
A21	121.34403
A22	120.07011
A23	130.79616
A24	117.14502
A25	120.90343
A26	120.21427
A27	119.24834
A28	124.32589

A29	90.25627
A30	118.32656
A31	120.65049
A32	120.21106
A33	119.69795
A34	120.06987
A35	122.42573
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A40	115.38107
A41	125.97288
A42	126.0339
A43	125.95919
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A45	118.01896
A46	125.76659
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A48	125.99134
A49	126.28045
A50	119.05938
A51	118.71825
A52	110.76152
A53	110.11047
A54	110.72745
A55	109.9823
A56	110.3726
A57	110.50114
A58	111.54358
A59	111.05864
A60	110.41238
A61	119.72585
A62	119.90074
A63	120.13227
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A65	119.57945
A66	119.64592
A67	119.94091
A68	120.15675
A69	119.56241
A70	119.22851
A71	118.24943
A72	119.89229
A73	121.83753
A74	120.44705
A75	118.00828
D1	-102.54382
D2	-50.46811
D3	66.65912
D4	1.19949
D5	0.55239
D6	-103.79982
D7	155.83773
D8	65.43269
D9	2.09191
D10	-2.3197

D11	33.28343
D12	-149.2793
D13	-13.42996
D14	-110.94885
D15	-179.90674
D16	2.32495
D17	-1.22117
D18	-0.59601
D19	0.62613
D20	177.66283
D21	-178.82412
D22	20.08029
D23	170.19748
D24	175.95952
D25	-1.20954
D26	0.72668
D27	-14.84171
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D29	88.13965
D30	-174.78409
D31	-0.19276
D32	-1.53458
D33	1.15597
D34	15.48026
D35	166.81698
D36	-0.36848
D37	1.34126
D38	-177.44495
D39	59.35686
D40	-113.09021
D41	-178.52894
D42	-179.13138
D43	178.13604
D44	153.98102
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D50	179.36367
D51	162.52238
D52	43.20446
D53	-76.3939
D54	14.22523
D55	-105.26407
D56	133.99572
D57	-0.22962
D58	-121.89919
D59	119.64868
D60	-3.3306
D61	-180.
D62	179.91455
D63	179.29944
D64	5.18721
D65	5.13028
D66	-179.96335
D67	178.74684

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 D68               -178.76599
 D69               -178.99517
 D70                -13.24123
 D71                179.3352
 D72               -177.72237
 D73                178.25824
 D74                 13.31949

Stoichiometry    C38H36NPZr
Framework group  C1[X(C38H36NPZr)]
Deg. of freedom   225
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1         40             0        1.172019   -1.346877    0.049790
   2         15             0       -2.271721   -0.264312    1.099908
   3          7             0        3.313058   -0.207181   -0.284073
   4          6             0        0.535664   -2.767626    2.058659
   5          6             0        1.776515   -3.270858    1.645979
   6          6             0        2.737169   -2.282218    1.867361
   7          6             0        2.083647   -1.162777    2.450833
   8          6             0        0.738045   -1.484140    2.590381
   9          6             0        2.016603   -2.634601   -2.007614
  10          6             0        1.128702   -3.498686   -1.388433
  11          6             0       -0.157936   -2.938840   -1.455749
  12          6             0       -0.055174   -1.732132   -2.172760
  13          6             0        1.284307   -1.529919   -2.493135
  14          6             0       -0.665234   -0.157346    0.337695
  15          6             0        0.273403    0.708285    0.026360
  16          6             0        0.349373    2.187001   -0.038552
  17          6             0        0.469054    2.847802   -1.274196
  18          6             0        0.540241    4.238469   -1.303707
  19          6             0        0.544745    5.002367   -0.149281
  20          6             0        0.448795    4.334356    1.065072
  21          6             0        0.339148    2.955788    1.139458
  22          6             0        0.508206    2.066361   -2.555697
  23          6             0        0.675668    6.513248   -0.203024
  24          6             0        0.211325    2.280824    2.478062
  25          6             0       -3.372466    1.054426    0.437299
  26          6             0       -4.683506    1.080686    0.903285
  27          6             0       -5.551995    2.084909    0.521963
  28          6             0       -5.120203    3.097958   -0.313753
  29          6             0       -3.820451    3.084756   -0.772192
  30          6             0       -2.955580    2.066510   -0.405790
  31          6             0       -2.998394   -1.742932    0.270708
  32          6             0       -3.106450   -2.921969    1.000116
  33          6             0       -3.545790   -4.093318    0.393120
  34          6             0       -3.883114   -4.097330   -0.938999
  35          6             0       -3.813837   -2.916409   -1.671069
  36          6             0       -3.385635   -1.753451   -1.067180
  37          6             0        3.487105    1.094326   -0.004283
  38          6             0        4.734881    1.686561    0.066852
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   39          6             0        5.859767    0.943667   -0.143928
   40          6             0        5.695012   -0.390779   -0.453118
   41          6             0        4.426750   -0.914584   -0.510732
   42          1             0       -0.299235   -3.219570    1.990694
   43          1             0        1.935744   -4.137287    1.274661
   44          1             0        3.663563   -2.345674    1.660310
   45          1             0        2.496798   -0.337854    2.696933
   46          1             0        0.067927   -0.927949    2.976992
   47          1             0        2.953924   -2.769196   -2.096692
   48          1             0        1.352773   -4.330287   -0.983131
   49          1             0       -0.948135   -3.311009   -1.084122
   50          1             0       -0.773824   -1.158169   -2.403623
   51          1             0        1.645207   -0.782164   -2.954699
   52          1             0        0.581152    4.680839   -2.143788
   53          1             0        0.459689    4.844903    1.871499
   54          1             0        0.321138    2.630615   -3.301640
   55          1             0       -0.155900    1.367099   -2.538147
   56          1             0        1.361155    1.662830   -2.678133
   57          1             0        0.525837    6.824149   -1.099846
   58          1             0        1.550694    6.780255    0.064811
   59          1             0        0.036708    6.923434    0.369291
   60          1             0        0.222592    2.911059    3.189118
   61          1             0        0.918008    1.647642    2.613371
   62          1             0       -0.624599    1.787758    2.530639
   63          1             0       -4.983869    0.408178    1.497463
   64          1             0       -6.441148    2.088922    0.847644
   65          1             0       -5.717400    3.785726   -0.575622
   66          1             0       -3.519995    3.770540   -1.353514
   67          1             0       -2.065028    2.065131   -0.735208
   68          1             0       -2.876601   -2.927028    1.921818
   69          1             0       -3.616134   -4.890868    0.899783
   70          1             0       -4.165856   -4.901039   -1.356719
   71          1             0       -4.064237   -2.917653   -2.587181
   72          1             0       -3.356635   -0.951081   -1.574343
   73          1             0        2.715730    1.628561    0.150210
   74          1             0        4.808433    2.613270    0.258702
   75          1             0        6.722974    1.316135   -0.070135
   76          1             0        6.447417   -0.938892   -0.631699
   77          1             0        4.334592   -1.831598   -0.727483
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.1004076      0.0872924
0.0572575
 Standard basis: LANL2DZ (5D, 7F)
 There are   453 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   453 basis functions,  1181 primitive gaussians,   455 cartesian
basis functions
   144 alpha electrons      144 beta electrons
       nuclear repulsion energy      4830.7754987779 Hartrees.
 NAtoms=   77 NActive=   77 NUniq=   77 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=T
 One-electron integrals computed using PRISM.
   1 Symmetry operations used in ECPInt.
 ECPInt:  NShTT=   39060 NPrTT=  285099 LenC2=   34315 LenP2D=  130151.
 LDataN:  DoStor=F MaxTD1= 5 Len=  102
```

```
 LDataN:  DoStor=T MaxTD1= 5 Len=  102
 NBasis=   453 RedAO= T  NBF=   453
 NBsUse=   453 1.00D-06 NBFU=   453
 Defaulting to unpruned grid for atomic number  40.
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 2.43D-02 ExpMax= 5.91D+03 ExpMxC= 2.05D+02 IAcc=3 IRadAn=
5 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         5 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Defaulting to unpruned grid for atomic number  40.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-04 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-02.
 Requested convergence on             energy=1.00D-02.
 No special actions if energy rises.
 Defaulting to unpruned grid for atomic number  40.
 EnCoef did   100 forward-backward iterations
```

```
 SCF Done:  E(RB+HF-LYP) =  -1576.72610257     A.U. after    8 cycles
            Convg  =    0.4231D-04             -V/T =  2.0224
            S**2   =   0.0000

 **********************************************************************

           Population analysis using the SCF density.

 **********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -14.38343 -10.24751 -10.24130 -10.22791 -
10.21980
 Alpha  occ. eigenvalues --  -10.21572 -10.18024 -10.17578 -10.17460 -
10.17373
 Alpha  occ. eigenvalues --  -10.17314 -10.17214 -10.17188 -10.17159 -
10.17065
```

```
 Alpha  occ. eigenvalues --  -10.17023 -10.16912 -10.16819 -10.16727 -
10.16603
 Alpha  occ. eigenvalues --  -10.16465 -10.16416 -10.16297 -10.16284 -
10.16258
 Alpha  occ. eigenvalues --  -10.16224 -10.16122 -10.16094 -10.16067 -
10.16029
 Alpha  occ. eigenvalues --  -10.15962 -10.15586 -10.14952 -10.14843 -
10.13797
 Alpha  occ. eigenvalues --  -10.13633 -10.13006 -10.12390 -10.12022  -
1.98976
 Alpha  occ. eigenvalues --   -1.20109  -1.18860  -1.18273  -1.00023  -
0.88544
 Alpha  occ. eigenvalues --   -0.87723  -0.86006  -0.85864  -0.85485  -
0.85023
 Alpha  occ. eigenvalues --   -0.81757  -0.78849  -0.78306  -0.76958  -
0.75807
 Alpha  occ. eigenvalues --   -0.74843  -0.74590  -0.72947  -0.72435  -
0.72160
 Alpha  occ. eigenvalues --   -0.71848  -0.71588  -0.71436  -0.69194  -
0.69012
 Alpha  occ. eigenvalues --   -0.68896  -0.68315  -0.64369  -0.62426  -
0.61578
 Alpha  occ. eigenvalues --   -0.60595  -0.59985  -0.58319  -0.57597  -
0.56921
 Alpha  occ. eigenvalues --   -0.56780  -0.56204  -0.56154  -0.55832  -
0.55588
 Alpha  occ. eigenvalues --   -0.55096  -0.53864  -0.53773  -0.52898  -
0.52847
 Alpha  occ. eigenvalues --   -0.50922  -0.48507  -0.47961  -0.47765  -
0.47101
 Alpha  occ. eigenvalues --   -0.46417  -0.44840  -0.44440  -0.44261  -
0.43969
 Alpha  occ. eigenvalues --   -0.43481  -0.43288  -0.42786  -0.42404  -
0.42310
 Alpha  occ. eigenvalues --   -0.41896  -0.41616  -0.41452  -0.41385  -
0.40955
 Alpha  occ. eigenvalues --   -0.40839  -0.40723  -0.40398  -0.40321  -
0.39891
 Alpha  occ. eigenvalues --   -0.39535  -0.39384  -0.38227  -0.38100  -
0.37854
 Alpha  occ. eigenvalues --   -0.37693  -0.36867  -0.36734  -0.36199  -
0.35757
 Alpha  occ. eigenvalues --   -0.35380  -0.35092  -0.34297  -0.33341  -
0.33056
 Alpha  occ. eigenvalues --   -0.32830  -0.32617  -0.32232  -0.31817  -
0.30143
 Alpha  occ. eigenvalues --   -0.29095  -0.27111  -0.25497  -0.25187  -
0.24922
 Alpha  occ. eigenvalues --   -0.24485  -0.23835  -0.23455  -0.22965  -
0.22387
 Alpha  occ. eigenvalues --   -0.21479  -0.20647  -0.18559  -0.16703
 Alpha virt. eigenvalues --   -0.06792  -0.04456  -0.00516  -0.00418
0.00175
 Alpha virt. eigenvalues --    0.00626   0.00941   0.01567   0.01758
0.02074
 Alpha virt. eigenvalues --    0.02328   0.02995   0.03301   0.03385
0.04375
```

```
 Alpha virt. eigenvalues --    0.05700   0.06856   0.08014   0.08530
0.08802
 Alpha virt. eigenvalues --    0.09340   0.10519   0.10658   0.12101
0.12480
 Alpha virt. eigenvalues --    0.12913   0.13466   0.13671   0.14127
0.14273
 Alpha virt. eigenvalues --    0.14681   0.15004   0.15534   0.15832
0.16233
 Alpha virt. eigenvalues --    0.16363   0.16810   0.17088   0.17368
0.17594
 Alpha virt. eigenvalues --    0.17906   0.18162   0.18199   0.18547
0.19015
 Alpha virt. eigenvalues --    0.19632   0.19761   0.19984   0.20284
0.20323
 Alpha virt. eigenvalues --    0.20803   0.20933   0.21407   0.22014
0.22288
 Alpha virt. eigenvalues --    0.22630   0.22975   0.23345   0.23413
0.23808
 Alpha virt. eigenvalues --    0.24031   0.24297   0.24607   0.25132
0.25313
 Alpha virt. eigenvalues --    0.25953   0.26118   0.26502   0.26607
0.27178
 Alpha virt. eigenvalues --    0.27365   0.27480   0.27949   0.28461
0.28613
 Alpha virt. eigenvalues --    0.28878   0.29379   0.29907   0.30160
0.30405
 Alpha virt. eigenvalues --    0.30512   0.30761   0.31088   0.31328
0.31515
 Alpha virt. eigenvalues --    0.31791   0.32165   0.32423   0.32780
0.32898
 Alpha virt. eigenvalues --    0.33120   0.33551   0.33892   0.34090
0.34285
 Alpha virt. eigenvalues --    0.34704   0.34886   0.34922   0.35363
0.35699
 Alpha virt. eigenvalues --    0.35950   0.35994   0.36130   0.36418
0.36733
 Alpha virt. eigenvalues --    0.37042   0.37449   0.38061   0.38425
0.38576
 Alpha virt. eigenvalues --    0.39157   0.39495   0.39855   0.39910
0.40183
 Alpha virt. eigenvalues --    0.40530   0.40654   0.41131   0.41275
0.41483
 Alpha virt. eigenvalues --    0.41667   0.41730   0.41830   0.42246
0.42403
 Alpha virt. eigenvalues --    0.43085   0.43221   0.43331   0.43887
0.44195
 Alpha virt. eigenvalues --    0.44337   0.44520   0.44653   0.45014
0.45139
 Alpha virt. eigenvalues --    0.45569   0.45854   0.46008   0.46165
0.46567
 Alpha virt. eigenvalues --    0.46976   0.47186   0.47488   0.47635
0.47837
 Alpha virt. eigenvalues --    0.48289   0.48648   0.48817   0.49437
0.49888
 Alpha virt. eigenvalues --    0.50295   0.50609   0.51028   0.51551
0.51866
```

```
 Alpha virt. eigenvalues --    0.52607   0.53000   0.53475   0.53766
0.54131
 Alpha virt. eigenvalues --    0.54389   0.54961   0.55203   0.55726
0.56181
 Alpha virt. eigenvalues --    0.57376   0.57637   0.58149   0.58385
0.58568
 Alpha virt. eigenvalues --    0.59141   0.59920   0.60163   0.60938
0.61498
 Alpha virt. eigenvalues --    0.62292   0.62532   0.63318   0.63560
0.64195
 Alpha virt. eigenvalues --    0.64404   0.64674   0.65271   0.65556
0.65951
 Alpha virt. eigenvalues --    0.66564   0.66726   0.67200   0.67635
0.68515
 Alpha virt. eigenvalues --    0.68765   0.69062   0.69238   0.69760
0.69850
 Alpha virt. eigenvalues --    0.70491   0.71384   0.71598   0.71822
0.72399
 Alpha virt. eigenvalues --    0.73040   0.73558   0.73946   0.74223
0.74892
 Alpha virt. eigenvalues --    0.75635   0.76065   0.76456   0.76953
0.77108
 Alpha virt. eigenvalues --    0.77352   0.77916   0.78252   0.78891
0.79397
 Alpha virt. eigenvalues --    0.80665   0.81460   0.82002   0.83058
0.83785
 Alpha virt. eigenvalues --    0.85291   0.86065   0.86749   0.87020
0.88296
 Alpha virt. eigenvalues --    0.90798   0.91130   0.92184   0.94778
0.95603
 Alpha virt. eigenvalues --    0.96416   0.98763   1.01515   1.02625
1.05905
 Alpha virt. eigenvalues --    1.08640   1.09472   1.11588   1.13046
1.14113
 Alpha virt. eigenvalues --    1.15330   1.15497   1.16471   1.18078
1.18418
 Alpha virt. eigenvalues --    1.20921   1.21306   1.22186   1.23213
1.24284
 Alpha virt. eigenvalues --    1.25367   1.25983   1.26468   1.27143
1.27386
 Alpha virt. eigenvalues --    1.28255   1.29294   1.29675   1.30478
1.30872
 Alpha virt. eigenvalues --    1.31833   1.32385   1.33312   1.34112
1.34879
 Alpha virt. eigenvalues --    1.35930   1.36510   1.37499   1.38270
1.39002
 Alpha virt. eigenvalues --    1.39065   1.39851   1.39936   1.40818
1.42333
 Alpha virt. eigenvalues --    1.43007   1.44086   1.44595   1.45510
1.47116
 Alpha virt. eigenvalues --    1.48022   1.48956   1.49632   1.50414
1.51629
 Alpha virt. eigenvalues --    1.51916   1.53941   1.55012   1.56318
1.57748
 Alpha virt. eigenvalues --    1.58468   1.59402   1.59897   1.60532
1.62050
```

```
 Alpha virt. eigenvalues --    1.62201   1.63250   1.63953   1.64593
1.65792
 Alpha virt. eigenvalues --    1.69183   1.69747   1.70034   1.72153
1.78919
 Alpha virt. eigenvalues --    1.82286   1.85871  14.58074  19.13425
          Condensed to atoms (all electrons):
 Mulliken atomic charges:
              1
     1  Zr   1.087319
     2  P    0.622480
     3  N   -0.179505
     4  C   -0.399523
     5  C   -0.375658
     6  C   -0.386456
     7  C   -0.418173
     8  C   -0.335093
     9  C   -0.393662
    10  C   -0.394320
    11  C   -0.385513
    12  C   -0.330910
    13  C   -0.404553
    14  C   -0.601342
    15  C   -0.346443
    16  C   -0.039863
    17  C    0.252008
    18  C   -0.767547
    19  C    0.423230
    20  C   -0.714656
    21  C    0.288179
    22  C   -0.875834
    23  C   -0.835297
    24  C   -0.902297
    25  C   -0.200474
    26  C   -0.337242
    27  C   -0.299615
    28  C   -0.317735
    29  C   -0.318364
    30  C   -0.298019
    31  C   -0.196750
    32  C   -0.407281
    33  C   -0.297546
    34  C   -0.313731
    35  C   -0.295434
    36  C   -0.292949
    37  C   -0.276729
    38  C   -0.290727
    39  C   -0.264191
    40  C   -0.295190
    41  C   -0.282293
    42  H    0.375321
    43  H    0.349441
    44  H    0.354088
    45  H    0.352400
    46  H    0.381458
    47  H    0.340583
    48  H    0.354673
    49  H    0.390375
```

```
    50  H    0.366952
    51  H    0.353773
    52  H    0.323394
    53  H    0.317007
    54  H    0.257677
    55  H    0.267551
    56  H    0.270192
    57  H    0.243317
    58  H    0.255875
    59  H    0.252473
    60  H    0.263857
    61  H    0.267525
    62  H    0.287672
    63  H    0.309543
    64  H    0.292324
    65  H    0.297095
    66  H    0.300046
    67  H    0.340118
    68  H    0.328246
    69  H    0.297319
    70  H    0.299082
    71  H    0.295986
    72  H    0.333817
    73  H    0.388730
    74  H    0.318673
    75  H    0.325470
    76  H    0.313254
    77  H    0.332390
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
     1  Zr   1.087319
     2  P    0.622480
     3  N   -0.179505
     4  C   -0.024203
     5  C   -0.026217
     6  C   -0.032369
     7  C   -0.065773
     8  C    0.046365
     9  C   -0.053079
    10  C   -0.039647
    11  C    0.004862
    12  C    0.036042
    13  C   -0.050780
    14  C   -0.601342
    15  C   -0.346443
    16  C   -0.039863
    17  C    0.252008
    18  C   -0.444152
    19  C    0.423230
    20  C   -0.397649
    21  C    0.288179
    22  C   -0.080414
    23  C   -0.083632
    24  C   -0.083243
    25  C   -0.200474
    26  C   -0.027699
```

```
   27  C   -0.007290
   28  C   -0.020639
   29  C   -0.018318
   30  C    0.042099
   31  C   -0.196750
   32  C   -0.079035
   33  C   -0.000227
   34  C   -0.014649
   35  C    0.000551
   36  C    0.040868
   37  C    0.112001
   38  C    0.027947
   39  C    0.061278
   40  C    0.018064
   41  C    0.050097
   42  H    0.000000
   43  H    0.000000
   44  H    0.000000
   45  H    0.000000
   46  H    0.000000
   47  H    0.000000
   48  H    0.000000
   49  H    0.000000
   50  H    0.000000
   51  H    0.000000
   52  H    0.000000
   53  H    0.000000
   54  H    0.000000
   55  H    0.000000
   56  H    0.000000
   57  H    0.000000
   58  H    0.000000
   59  H    0.000000
   60  H    0.000000
   61  H    0.000000
   62  H    0.000000
   63  H    0.000000
   64  H    0.000000
   65  H    0.000000
   66  H    0.000000
   67  H    0.000000
   68  H    0.000000
   69  H    0.000000
   70  H    0.000000
   71  H    0.000000
   72  H    0.000000
   73  H    0.000000
   74  H    0.000000
   75  H    0.000000
   76  H    0.000000
   77  H    0.000000
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>= 19053.1575
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     6.4555    Y=     0.5296    Z=    -1.4051  Tot=     6.6278
Quadrupole moment (field-independent basis, Debye-Ang):
```

```
   XX=  -219.6272   YY=  -245.7039   ZZ=  -267.3599
   XY=     6.2978   XZ=    -1.0880   YZ=    -1.0462
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=    24.6031   YY=    -1.4736   ZZ=   -23.1296
   XY=     6.2978   XZ=    -1.0880   YZ=    -1.0462
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=   274.7313  YYY=   -21.5862  ZZZ=   -16.7861  XYY=     5.8487
  XXY=     1.4146  XXZ=   -21.0752  XZZ=   -14.7387  YZZ=    32.9273
  YYZ=    -4.2525  XYZ=    19.2078
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=-11025.1532 YYYY=-10298.8108 ZZZZ= -3165.9725 XXXY=  -133.3964
 XXXZ=  -141.9099 YYYX=   133.1028 YYYZ=   -71.9189 ZZZX=    -1.1022
 ZZZY=     7.2818 XXYY= -3660.0924 XXZZ= -2687.2705 YYZZ= -2376.0631
 XXYZ=    77.4101 YYXZ=    46.2660 ZZXY=    97.8324
 N-N= 4.830775498778D+03 E-N=-1.330650103667D+04  KE=
1.542174195549D+03
 Evaluate density.
 Using the total density.
 Monte-Carlo method of calculating molar volume:
 based on  0.001 e/bohr**3 density envelope.
 Number of points per bohr**3 =  100 CutOff= 1.00D-04
 Using the SCF density.
 There are      3074 points.  Will hold      3074 in memory.
 LenV=   132600191 MDV=   134217728.
 Box volume =29052.036 fraction occupied=0.149
 Integrated density= 2.391051303608108OD+02 error=-
4.8894869639189213D+01
 Molar volume = 4328.508 bohr**3/mol (386.271 cm**3/mol)
 Recommended a0 for SCRF calculation =  6.39 angstrom ( 12.07 bohr)
 1\1\GINC-BEDROCK04\SP\RB3LYP\LANL2DZ\C38H36N1P1Zr1\JAMIN\30-Apr-2008\0
 \\# volume=tight b3lyp/lanl2dz geom=connectivity\\volume calc for mono
 mer\\0,1\Zr\P,1,3.7595267\N,1,2.44834951,2,134.83580428\C,1,2.54146165
 ,3,125.94245385,2,-102.54382365,0\C,4,1.40116326,1,75.29931727,3,-50.4
 6810682,0\C,5,1.39616382,4,107.95800745,1,66.65911811,0\C,6,1.42150561
 ,5,107.84204775,4,1.19948987,0\C,7,1.39046478,6,107.70359408,5,0.55239
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 75.16915115,3,155.83773482,0\C,10,1.40477638,9,108.487339,1,65.4326916
 1,0\C,11,1.40741154,10,107.41168203,9,2.09190997,0\C,12,1.39202703,11,
 108.18340556,10,-2.31970221,0\C,2,1.78135057,1,21.82679543,3,33.283426
 27,0\C,14,1.3142629,2,141.72042324,1,-149.27930154,0\C,15,1.48208827,1
 4,134.75918753,2,-13.42995969,0\C,16,1.40634141,15,120.77357293,14,-11
 0.94885146,0\C,17,1.39280035,16,119.47992669,15,-179.90674486,0\C,18,1
 .38429005,17,122.24125034,16,2.32494618,0\C,19,1.3892803,18,117.605359
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 ,17,1.50147491,16,120.50241712,15,0.62612976,0\C,19,1.51749452,18,121.
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 2,117.14502214,1,170.19747888,0\C,26,1.38135605,25,120.9034269,2,175.9
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 9492,27,119.2483388,26,0.72668063,0\C,25,1.38163224,2,124.3258925,1,-1
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 62592,2,118.32655547,1,88.13965232,0\C,32,1.39051142,31,120.65049024,2
 ,-174.78408837,0\C,33,1.37417101,32,120.21106463,31,-0.19275872,0\C,34
 ,1.39114978,33,119.69795192,32,-1.5345835,0\C,35,1.3785903,34,120.0698
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 37,1.38302084,3,122.8744313,1,166.81697615,0\C,38,1.36443675,37,120.17
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\C,3,1.33869497,1,120.30545918,14,-177.4449539,0\H,4,0.95180412,1,115.
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,0\H,9,0.95111561,1,118.01895578,14,153.98102396,0\H,10,0.95186063,9,1
25.76659008,1,-114.38637048,0\H,11,0.94922613,10,125.97574978,9,-177.9
3006764,0\H,12,0.94825618,11,125.99133767,10,177.2933478,0\H,13,0.9499
6266,12,126.28044521,11,-178.21993574,0\H,18,0.9503169,17,119.0593777,
16,-177.24227814,0\H,20,0.95451643,19,118.71824566,18,179.36367157,0\H
,22,0.95383817,17,110.76151948,16,162.52238285,0\H,22,0.96452675,17,11
0.11046978,16,43.20445794,0\H,22,0.95149916,17,110.72745221,16,-76.393
90013,0\H,23,0.96093647,19,109.98230291,18,14.22522705,0\H,23,0.953257
21,19,110.37259806,18,-105.26406775,0\H,23,0.95082382,19,110.50114325,
18,133.995724,0\H,24,0.95022371,21,111.54358155,20,-0.22962475,0\H,24,
0.95845086,21,111.05863924,20,-121.89918511,0\H,24,0.97192954,21,110.4
123766,20,119.64867724,0\H,26,0.94632635,25,119.72584993,2,-3.33059595
,0\H,27,0.94693048,26,119.90074147,25,-180.,0\H,28,0.94775821,27,120.1
3227082,26,179.91454694,0\H,29,0.94789655,28,119.73318088,27,179.29944
046,0\H,30,0.9495263,25,119.57944865,2,5.18720925,0\H,32,0.94994299,31
,119.64591741,2,5.13027919,0\H,33,0.9474919,32,119.94090817,31,-179.96
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748,34,119.5624072,33,-178.76598723,0\H,36,0.94965932,35,119.22851271,
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8,0.94921316,37,119.89228766,3,179.33519596,0\H,39,0.94302883,38,121.8
3752699,37,-177.72236771,0\H,40,0.94785647,39,120.44704739,38,178.2582
4312,0\H,41,0.9467781,3,118.00828327,1,13.31948504,0\\Version=IA32L-G0
3RevD.01\State=1-A\HF=-1576.7261026\RMSD=4.231e-05\Thermal=0.\Dipole=0
.9680546,-0.0425334,-2.4208536\PG=C01 [X(C38H36N1P1Zr1)]\\@

HE WHO LOVES TO READ, AND KNOWS HOW TO REFLECT,
HAS LAID BY A PERPETUAL FEAST FOR HIS OLD AGE.
-- UNCLE ESEK, "SCRIBNER'S MONTHLY", SEPT. 1880
Job cpu time: 0 days 3 hours 0 minutes 53.4 seconds.
File lengths (MBytes): RWF=   119 Int=   0 D2E=   0 Chk=
16 Scr=   1
Normal termination of Gaussian 03 at Wed Apr 30 21:00:50 2008.

X-Ray Structural Data for 1:

Data Collection

A fragment of a yellow plate-like crystal of C48 H58 P2 Zr2 having approximate dimensions of .4 x .1 x .1 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a CCD area detector [10] CCD area detector with graphite monochromated MoKradiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 3840 centered reflections with I > $10\sigma(I)$ in the range $3.41 < \theta < 24.71^{o}$ corresponded to a C-centered Monoclinic cell with dimensions:

a = 22.707(3) Å	$\alpha = 90^{o}$
b = 9.364(1) Å	$\beta = 112.552(2)^{o}$
c = 21.053(3) Å	$\gamma = 90^{o}$
V = 8876(1) $Å^3$	

For Z = 4 and F.W. = 879.32, the calculated density is 1.413 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

C2/c

The data were collected at a temperature of 173(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3^{o} counted for a total of 30 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[11] to a maximum θ value of 24.71^{o}. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 1.0000, Tmin = 0.8719). Of the 9052 reflections that were collected, 3487 were unique (R_{int} = 0.0498); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the

rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 3487 reflections (all data) and 235 variable parameters and converged (largest parameter shift was 0.000 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0315 \text{ for } 2624 \text{ data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.0774$$

The standard deviation of an observation of unit weight[4] was 0.907. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.667 and -0.423 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[9] crystallographic software package of Bruker Analytical X-ray Systems Inc.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C48 H58 P2 Zr2
Formula Weight	879.32
Crystal Color, Habit	yellow, plate
Crystal Dimensions	.4 x .1 x .1 mm
Crystal System	Monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 22.707(3) Å
	b = 9.364(1) Å
	c = 21.053(3) Å
	α= 90 ^{o}
	β= 112.552(2) ^{o}
	γ = 90^o
	V = 4134.2(10) $Å^3$
Space Group	C2/c
Z value	4
D_{calc}	1.413 g/cm^3

F_{000}	1824
μ(MoK)	0.61 cm^{-1}

B. Intensity Measurements

Diffractometer	CCD area detector
Radiation	MoK(λ = 0.71073 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	30 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
θ_{max}	24.71°
No. of Reflections Measured	Total: 9052 Unique: 3487 (R_{int} = 0.0498)
Corrections	Lorentz-polarization Absorption (Tmax = 1.0000, Tmin = 0.8719)

C. Structure Solution and Refinement

Structure Solution	direct (SHELXS-97 (Sheldrick, 1990))
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|F_o\|^2 - \|F_c\|^2)^2$
Least Squares Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (qP)^2 + 0.000P]$ where $P = [F_o^2 + 2F_c^2]/3$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	2624
No. Variables	235
Residuals: R; wR_2; Rall	0.0315; 0.0774; 0.0444
Goodness of Fit Indicator	0.907
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.667 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.423 $e^-/Å^3$

Table 1. Atomic coordinates and U_{iso}/U_{eq} and occupancy

atom	x	y	z	U_{eq}	Occupancy
Zr1	0.1105(1)	0.3736(1)	0.2417(1)	0.020(1)	1
P2	-0.0036(1)	0.2469(1)	0.1549(1)	0.020(1)	1
C1	0.2284(2)	0.3141(4)	0.2929(2)	0.041(1)	1
C2	0.2114(2)	0.3188(4)	0.2215(2)	0.040(1)	1
C3	0.1702(2)	0.2061(4)	0.1924(2)	0.036(1)	1
C4	0.1632(2)	0.1269(4)	0.2459(2)	0.034(1)	1
C5	0.1999(2)	0.1942(4)	0.3078(2)	0.037(1)	1
C6	0.1257(2)	0.5758(4)	0.1654(2)	0.042(1)	1
C7	0.0609(2)	0.5588(3)	0.1463(2)	0.031(1)	1
C8	0.0441(2)	0.5963(3)	0.2008(2)	0.027(1)	1
C9	0.0998(2)	0.6379(3)	0.2563(2)	0.034(1)	1
C10	0.1508(2)	0.6218(4)	0.2338(2)	0.044(1)	1
C11	0.0656(1)	0.3135(3)	0.3190(1)	0.020(1)	1
C12	0.1147(1)	0.3969(3)	0.3483(1)	0.022(1)	1
C13	0.1504(1)	0.4712(3)	0.4132(1)	0.024(1)	1
C14	0.1262(2)	0.5894(3)	0.4354(2)	0.030(1)	1
C15	0.1617(2)	0.6601(4)	0.4960(2)	0.037(1)	1
C16	0.2227(2)	0.6143(4)	0.5363(2)	0.039(1)	1
C17	0.2475(2)	0.4997(4)	0.5149(2)	0.041(1)	1
C18	0.2125(2)	0.4289(4)	0.4542(2)	0.033(1)	1
C19	-0.0043(2)	0.0478(3)	0.1646(1)	0.027(1)	1
C20	0.0296(2)	-0.0319(3)	0.1254(2)	0.038(1)	1
C21	-0.0697(2)	-0.0181(4)	0.1505(2)	0.037(1)	1
C22	-0.0327(1)	0.2807(3)	0.0604(1)	0.025(1)	1
C23	-0.0928(2)	0.1988(4)	0.0149(2)	0.038(1)	1
C24	0.0197(2)	0.2673(4)	0.0321(1)	0.033(1)	1

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr1	0.018(1)	0.022(1)	0.020(1)	0.003(1)	0.007(1)	0.004(1)
P2	0.025(1)	0.018(1)	0.016(1)	0.000(1)	0.007(1)	0.001(1)
C1	0.021(2)	0.053(2)	0.042(2)	-0.003(2)	0.004(2)	0.015(2)
C2	0.024(2)	0.050(2)	0.051(2)	0.006(2)	0.020(2)	0.014(2)
C3	0.036(2)	0.043(2)	0.029(2)	0.003(2)	0.014(2)	0.021(2)
C4	0.031(2)	0.032(2)	0.038(2)	0.006(2)	0.014(2)	0.019(2)
C5	0.032(2)	0.048(2)	0.029(2)	0.009(2)	0.010(2)	0.029(2)
C6	0.049(2)	0.037(2)	0.050(2)	0.020(2)	0.031(2)	0.008(2)
C7	0.035(2)	0.022(2)	0.031(2)	0.013(1)	0.008(2)	0.002(2)
C8	0.022(2)	0.016(2)	0.044(2)	0.012(1)	0.012(2)	0.007(1)
C9	0.047(2)	0.019(2)	0.033(2)	0.000(1)	0.013(2)	-0.002(2)
C10	0.026(2)	0.034(2)	0.064(2)	0.011(2)	0.006(2)	-0.012(2)
C11	0.019(2)	0.019(2)	0.019(1)	0.004(1)	0.006(1)	0.005(1)
C12	0.017(2)	0.020(2)	0.023(2)	0.001(1)	0.003(1)	0.006(1)
C13	0.021(2)	0.028(2)	0.021(2)	0.000(1)	0.007(1)	-0.004(1)
C14	0.024(2)	0.035(2)	0.030(2)	-0.004(1)	0.009(1)	-0.006(1)
C15	0.038(2)	0.040(2)	0.038(2)	-0.015(2)	0.021(2)	-0.014(2)
C16	0.037(2)	0.052(2)	0.023(2)	-0.008(2)	0.005(2)	-0.015(2)
C17	0.029(2)	0.055(3)	0.027(2)	0.003(2)	-0.004(2)	-0.001(2)
C18	0.029(2)	0.039(2)	0.026(2)	0.001(2)	0.004(1)	0.005(2)
C19	0.042(2)	0.019(2)	0.018(2)	0.000(1)	0.009(1)	0.000(1)
C20	0.065(3)	0.021(2)	0.024(2)	-0.002(1)	0.014(2)	0.010(2)
C21	0.057(2)	0.025(2)	0.028(2)	-0.003(2)	0.014(2)	-0.011(2)
C22	0.031(2)	0.025(2)	0.019(2)	0.003(1)	0.009(1)	0.003(1)
C23	0.044(2)	0.042(2)	0.022(2)	-0.002(2)	0.005(2)	-0.001(2)
C24	0.045(2)	0.035(2)	0.022(2)	0.004(1)	0.016(2)	0.006(2)

The general temperature factor expression:

$$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Zr1	C12	2.219(3)	Zr1	C11	2.298(3)
Zr1	C9	2.518(3)	Zr1	C8	2.524(3)
Zr1	C10	2.527(3)	Zr1	C1	2.533(3)
Zr1	C2	2.538(3)	Zr1	C3	2.540(3)
Zr1	C7	2.566(3)	Zr1	C4	2.587(3)
Zr1	C5	2.591(3)	Zr1	C6	2.591(3)
P2	C11#1	1.806(3)	P2	C22	1.867(3)
P2	C19	1.876(3)	C1	C5	1.390(5)
C1	C2	1.402(5)	C1	H1A	0.9800
C2	C3	1.388(5)	C2	H2A	0.9800
C3	C4	1.407(5)	C3	H3A	0.9800
C4	C5	1.400(5)	C4	H4A	0.9800
C5	H5A	0.9800	C6	C7	1.378(4)
C6	C10	1.399(5)	C6	H6A	0.9800
C7	C8	1.386(4)	C7	H7A	0.9800
C8	C9	1.408(4)	C8	H8A	0.9800
C9	C10	1.416(5)	C9	H9A	0.9800
C10	H10A	0.9800	C11	C12	1.307(4)
C11	P2#1	1.806(3)	C12	C13	1.470(4)
C13	C14	1.394(4)	C13	C18	1.399(4)
C14	C15	1.388(4)	C14	H14A	0.9300
C15	C16	1.387(5)	C15	H15A	0.9300
C16	C17	1.366(5)	C16	H16A	0.9300
C17	C18	1.388(4)	C17	H17A	0.9300
C18	H18A	0.9300	C19	C20	1.522(4)
C19	C21	1.530(4)	C19	H19A	0.9800
C20	H20A	0.9600	C20	H20B	0.9600
C20	H20C	0.9600	C21	H21A	0.9600
C21	H21B	0.9600	C21	H21C	0.9600
C22	C24	1.528(4)	C22	C23	1.538(4)
C22	H22A	0.9800	C23	H23A	0.9600
C23	H23B	0.9600	C23	H23C	0.9600
C24	H24A	0.9600	C24	H24B	0.9600
C24	H24C	0.9600			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C12	Zr1	C11	33.57(10)	C12	Zr1	C9	75.43(11)
C11	Zr1	C9	93.70(11)	C12	Zr1	C8	92.98(10)
C11	Zr1	C8	94.28(10)	C9	Zr1	C8	32.44(10)
C12	Zr1	C10	95.72(12)	C11	Zr1	C10	122.83(12)
C9	Zr1	C10	32.61(11)	C8	Zr1	C10	53.20(11)
C12	Zr1	C1	87.87(11)	C11	Zr1	C1	109.17(11)
C9	Zr1	C1	107.45(12)	C8	Zr1	C1	136.23(12)
C10	Zr1	C1	83.14(12)	C12	Zr1	C2	119.87(11)
C11	Zr1	C2	138.08(11)	C9	Zr1	C2	110.78(12)
C8	Zr1	C2	124.70(11)	C10	Zr1	C2	78.60(13)
C1	Zr1	C2	32.11(11)	C12	Zr1	C3	130.63(10)
C11	Zr1	C3	126.13(11)	C9	Zr1	C3	138.47(12)
C8	Zr1	C3	135.50(10)	C10	Zr1	C3	106.15(12)
C1	Zr1	C3	52.87(11)	C2	Zr1	C3	31.72(11)
C12	Zr1	C7	124.12(10)	C11	Zr1	C7	122.64(10)
C9	Zr1	C7	52.90(10)	C8	Zr1	C7	31.60(10)
C10	Zr1	C7	52.24(11)	C1	Zr1	C7	123.84(11)
C2	Zr1	C7	99.14(11)	C3	Zr1	C7	103.90(10)
C12	Zr1	C4	102.34(10)	C11	Zr1	C4	94.72(10)
C9	Zr1	C4	159.87(11)	C8	Zr1	C4	163.19(10)
C10	Zr1	C4	130.53(12)	C1	Zr1	C4	52.45(12)
C2	Zr1	C4	52.43(12)	C3	Zr1	C4	31.85(10)
C7	Zr1	C4	133.53(11)	C12	Zr1	C5	78.47(10)
C11	Zr1	C5	86.00(10)	C9	Zr1	C5	131.65(12)
C8	Zr1	C5	164.09(11)	C10	Zr1	C5	113.79(12)
C1	Zr1	C5	31.46(11)	C2	Zr1	C5	52.22(11)
C3	Zr1	C5	52.28(10)	C7	Zr1	C5	151.35(11)
C4	Zr1	C5	31.37(10)	C12	Zr1	C6	126.21(11)
C11	Zr1	C6	145.00(11)	C9	Zr1	C6	53.07(11)
C8	Zr1	C6	52.29(11)	C10	Zr1	C6	31.70(12)
C1	Zr1	C6	93.13(12)	C2	Zr1	C6	72.56(12)
C3	Zr1	C6	88.80(11)	C7	Zr1	C6	30.99(10)
C4	Zr1	C6	120.27(11)	C5	Zr1	C6	122.95(12)
C11#1	P2	C22	105.42(13)	C11#1	P2	C19	105.66(14)
C22	P2	C19	105.67(13)	C11#1	P2	Zr1	106.86(9)
C22	P2	Zr1	119.02(10)	C19	P2	Zr1	113.21(10)
C5	C1	C2	107.9(3)	C5	C1	Zr1	76.56(18)
C2	C1	Zr1	74.12(18)	C5	C1	H1A	125.4
C2	C1	H1A	125.4	Zr1	C1	H1A	125.4

C3	C2	C1	108.1(3)	C3	C2	Zr1	74.24(18)
C1	C2	Zr1	73.77(19)	C3	C2	H2A	125.6
C1	C2	H2A	125.6	Zr1	C2	H2A	125.6
C2	C3	C4	108.2(3)	C2	C3	Zr1	74.04(18)
C4	C3	Zr1	75.89(18)	C2	C3	H3A	125.4
C4	C3	H3A	125.4	Zr1	C3	H3A	125.4
C5	C4	C3	107.3(3)	C5	C4	Zr1	74.49(19)
C3	C4	Zr1	72.27(18)	C5	C4	H4A	126.0
C3	C4	H4A	126.0	Zr1	C4	H4A	126.0
C1	C5	C4	108.4(3)	C1	C5	Zr1	71.99(18)
C4	C5	Zr1	74.15(18)	C1	C5	H5A	125.6
C4	C5	H5A	125.6	Zr1	C5	H5A	125.6
C7	C6	C10	107.7(3)	C7	C6	Zr1	73.48(18)
C10	C6	Zr1	71.62(19)	C7	C6	H6A	126.0
C10	C6	H6A	126.0	Zr1	C6	H6A	126.0
C6	C7	C8	109.3(3)	C6	C7	Zr1	75.52(18)
C8	C7	Zr1	72.54(16)	C6	C7	H7A	125.1
C8	C7	H7A	125.1	Zr1	C7	H7A	125.1
C7	C8	C9	108.2(3)	C7	C8	Zr1	75.85(17)
C9	C8	Zr1	73.53(17)	C7	C8	H8A	125.4
C9	C8	H8A	125.4	Zr1	C8	H8A	125.4
C8	C9	C10	106.4(3)	C8	C9	Zr1	74.02(17)
C10	C9	Zr1	74.04(19)	C8	C9	H9A	126.3
C10	C9	H9A	126.3	Zr1	C9	H9A	126.3
C6	C10	C9	108.4(3)	C6	C10	Zr1	76.7(2)
C9	C10	Zr1	73.34(18)	C6	C10	H10A	125.3
C9	C10	H10A	125.3	Zr1	C10	H10A	125.3
C12	C11	P2#1	133.4(2)	C12	C11	Zr1	69.87(17)
P2#1	C11	Zr1	155.36(15)	C11	C12	C13	141.9(3)
C11	C12	Zr1	76.55(17)	C13	C12	Zr1	141.4(2)
C14	C13	C18	116.8(3)	C14	C13	C12	122.7(3)
C18	C13	C12	120.4(3)	C15	C14	C13	121.6(3)
C15	C14	H14A	119.2	C13	C14	H14A	119.2
C16	C15	C14	120.4(3)	C16	C15	H15A	119.8
C14	C15	H15A	119.8	C17	C16	C15	118.9(3)
C17	C16	H16A	120.5	C15	C16	H16A	120.5
C16	C17	C18	121.1(3)	C16	C17	H17A	119.5
C18	C17	H17A	119.5	C17	C18	C13	121.2(3)
C17	C18	H18A	119.4	C13	C18	H18A	119.4
C20	C19	C21	110.6(3)	C20	C19	P2	113.7(2)
C21	C19	P2	115.3(2)	C20	C19	H19A	105.4
C21	C19	H19A	105.4	P2	C19	H19A	105.4
C19	C20	H20A	109.5	C19	C20	H20B	109.5
H20A	C20	H20B	109.5	C19	C20	H20C	109.5
H20A	C20	H20C	109.5	H20B	C20	H20C	109.5
C19	C21	H21A	109.5	C19	C21	H21B	109.5

H21A	C21	H21B	109.5	C19	C21	H21C	109.5
H21A	C21	H21C	109.5	H21B	C21	H21C	109.5
C24	C22	C23	110.7(2)	C24	C22	P2	113.0(2)
C23	C22	P2	116.5(2)	C24	C22	H22A	105.1
C23	C22	H22A	105.1	P2	C22	H22A	105.1
C22	C23	H23A	109.5	C22	C23	H23B	109.5
H23A	C23	H23B	109.5	C22	C23	H23C	109.5
H23A	C23	H23C	109.5	H23B	C23	H23C	109.5
C22	C24	H24A	109.5	C22	C24	H24B	109.5
H24A	C24	H24B	109.5	C22	C24	H24C	109.5
H24A	C24	H24C	109.5	H24B	C24	H24C	109.5

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C12	Zr1	P2	C11#1	36.70(13)	C11	Zr1	P2	C11#1	43.25(7)
C9	Zr1	P2	C11#1	-46.10(13)	C8	Zr1	P2	C11#1	-52.94(12)
C10	Zr1	P2	C11#1	-79.93(15)	C1	Zr1	P2	C11#1	149.66(16)
C2	Zr1	P2	C11#1	-177.69(14)	C3	Zr1	P2	C11#1	170.52(12)
C7	Zr1	P2	C11#1	-84.79(13)	C4	Zr1	P2	C11#1	138.70(12)
C5	Zr1	P2	C11#1	123.60(13)	C6	Zr1	P2	C11#1	-101.00(13)
C12	Zr1	P2	C22	155.77(13)	C11	Zr1	P2	C22	162.32(13)
C9	Zr1	P2	C22	72.98(14)	C8	Zr1	P2	C22	66.13(13)
C10	Zr1	P2	C22	39.14(16)	C1	Zr1	P2	C22	-91.27(17)
C2	Zr1	P2	C22	-58.62(15)	C3	Zr1	P2	C22	-70.41(13)
C7	Zr1	P2	C22	34.28(14)	C4	Zr1	P2	C22	-102.23(13)
C5	Zr1	P2	C22	-117.33(14)	C6	Zr1	P2	C22	18.07(14)
C12	Zr1	P2	C19	-79.20(13)	C11	Zr1	P2	C19	-72.66(12)
C9	Zr1	P2	C19	-162.00(13)	C8	Zr1	P2	C19	-168.85(13)
C10	Zr1	P2	C19	164.17(15)	C1	Zr1	P2	C19	33.76(17)
C2	Zr1	P2	C19	66.40(14)	C3	Zr1	P2	C19	54.62(13)
C7	Zr1	P2	C19	159.31(13)	C4	Zr1	P2	C19	22.80(12)
C5	Zr1	P2	C19	7.69(13)	C6	Zr1	P2	C19	143.10(13)
C12	Zr1	C1	C5	71.2(2)	C11	Zr1	C1	C5	44.8(2)
C9	Zr1	C1	C5	145.2(2)	C8	Zr1	C1	C5	163.27(18)
C10	Zr1	C1	C5	167.2(2)	C2	Zr1	C1	C5	-113.3(3)
C3	Zr1	C1	C5	-76.5(2)	C7	Zr1	C1	C5	-158.21(19)
C4	Zr1	C1	C5	-36.17(19)	C6	Zr1	C1	C5	-162.7(2)
C12	Zr1	C1	C2	-175.5(2)	C11	Zr1	C1	C2	158.1(2)
C9	Zr1	C1	C2	-101.5(2)	C8	Zr1	C1	C2	-83.4(3)
C10	Zr1	C1	C2	-79.5(2)	C3	Zr1	C1	C2	36.8(2)
C7	Zr1	C1	C2	-44.9(3)	C4	Zr1	C1	C2	77.2(2)
C5	Zr1	C1	C2	113.3(3)	C6	Zr1	C1	C2	-49.3(2)
C5	C1	C2	C3	2.9(4)	Zr1	C1	C2	C3	-66.9(2)
C5	C1	C2	Zr1	69.8(2)	C12	Zr1	C2	C3	119.9(2)
C11	Zr1	C2	C3	82.9(2)	C9	Zr1	C2	C3	-155.36(19)
C8	Zr1	C2	C3	-122.0(2)	C10	Zr1	C2	C3	-150.0(2)
C1	Zr1	C2	C3	114.7(3)	C7	Zr1	C2	C3	-101.7(2)
C4	Zr1	C2	C3	37.46(19)	C5	Zr1	C2	C3	77.4(2)
C6	Zr1	C2	C3	-117.8(2)	C12	Zr1	C2	C1	5.2(3)
C11	Zr1	C2	C1	-31.8(3)	C9	Zr1	C2	C1	89.9(2)
C8	Zr1	C2	C1	123.3(2)	C10	Zr1	C2	C1	95.3(2)
C3	Zr1	C2	C1	-114.7(3)	C7	Zr1	C2	C1	143.6(2)
C4	Zr1	C2	C1	-77.3(2)	C5	Zr1	C2	C1	-37.3(2)
C6	Zr1	C2	C1	127.5(3)	C1	C2	C3	C4	-2.3(4)

Zr1	C2	C3	C4	-68.8(2)	C1	C2	C3	Zr1	66.6(2)
C12	Zr1	C3	C2	-81.9(2)	C11	Zr1	C3	C2	-124.8(2)
C9	Zr1	C3	C2	36.0(3)	C8	Zr1	C3	C2	84.2(2)
C10	Zr1	C3	C2	30.7(2)	C1	Zr1	C3	C2	-37.3(2)
C7	Zr1	C3	C2	84.9(2)	C4	Zr1	C3	C2	-114.0(3)
C5	Zr1	C3	C2	-77.2(2)	C6	Zr1	C3	C2	57.6(2)
C12	Zr1	C3	C4	32.0(3)	C11	Zr1	C3	C4	-10.8(3)
C9	Zr1	C3	C4	150.00(19)	C8	Zr1	C3	C4	-161.84(19)
C10	Zr1	C3	C4	144.7(2)	C1	Zr1	C3	C4	76.7(2)
C2	Zr1	C3	C4	114.0(3)	C7	Zr1	C3	C4	-161.1(2)
C5	Zr1	C3	C4	36.8(2)	C6	Zr1	C3	C4	171.6(2)
C2	C3	C4	C5	0.8(3)	Zr1	C3	C4	C5	-66.8(2)
C2	C3	C4	Zr1	67.6(2)	C12	Zr1	C4	C5	-41.2(2)
C11	Zr1	C4	C5	-74.3(2)	C9	Zr1	C4	C5	40.1(4)
C8	Zr1	C4	C5	163.5(3)	C10	Zr1	C4	C5	67.5(3)
C1	Zr1	C4	C5	36.3(2)	C2	Zr1	C4	C5	77.1(2)
C3	Zr1	C4	C5	114.4(3)	C7	Zr1	C4	C5	140.1(2)
C6	Zr1	C4	C5	104.6(2)	C12	Zr1	C4	C3	-155.7(2)
C11	Zr1	C4	C3	171.2(2)	C9	Zr1	C4	C3	-74.4(4)
C8	Zr1	C4	C3	49.1(5)	C10	Zr1	C4	C3	-46.9(3)
C1	Zr1	C4	C3	-78.1(2)	C2	Zr1	C4	C3	-37.3(2)
C7	Zr1	C4	C3	25.7(3)	C5	Zr1	C4	C3	-114.4(3)
C6	Zr1	C4	C3	-9.8(2)	C2	C1	C5	C4	-2.4(4)
Zr1	C1	C5	C4	65.7(2)	C2	C1	C5	Zr1	-68.1(2)
C3	C4	C5	C1	1.0(4)	Zr1	C4	C5	C1	-64.3(2)
C3	C4	C5	Zr1	65.3(2)	C12	Zr1	C5	C1	-105.1(2)
C11	Zr1	C5	C1	-138.2(2)	C9	Zr1	C5	C1	-46.8(3)
C8	Zr1	C5	C1	-46.6(5)	C10	Zr1	C5	C1	-13.9(2)
C2	Zr1	C5	C1	38.1(2)	C3	Zr1	C5	C1	78.6(2)
C7	Zr1	C5	C1	40.0(3)	C4	Zr1	C5	C1	116.0(3)
C6	Zr1	C5	C1	20.8(3)	C12	Zr1	C5	C4	138.9(2)
C11	Zr1	C5	C4	105.9(2)	C9	Zr1	C5	C4	-162.76(19)
C8	Zr1	C5	C4	-162.6(3)	C10	Zr1	C5	C4	-129.9(2)
C1	Zr1	C5	C4	-116.0(3)	C2	Zr1	C5	C4	-77.8(2)
C3	Zr1	C5	C4	-37.4(2)	C7	Zr1	C5	C4	-76.0(3)
C6	Zr1	C5	C4	-95.2(2)	C12	Zr1	C6	C7	-97.5(2)
C11	Zr1	C6	C7	-56.5(3)	C9	Zr1	C6	C7	-77.6(2)
C8	Zr1	C6	C7	-36.52(19)	C10	Zr1	C6	C7	-115.6(3)
C1	Zr1	C6	C7	172.8(2)	C2	Zr1	C6	C7	147.8(2)
C3	Zr1	C6	C7	120.1(2)	C4	Zr1	C6	C7	125.3(2)
C5	Zr1	C6	C7	162.14(19)	C12	Zr1	C6	C10	18.1(3)
C11	Zr1	C6	C10	59.1(3)	C9	Zr1	C6	C10	38.0(2)
C8	Zr1	C6	C10	79.1(2)	C1	Zr1	C6	C10	-71.6(2)
C2	Zr1	C6	C10	-96.6(2)	C3	Zr1	C6	C10	-124.3(2)
C7	Zr1	C6	C10	115.6(3)	C4	Zr1	C6	C10	-119.1(2)
C5	Zr1	C6	C10	-82.3(2)	C10	C6	C7	C8	1.3(4)

Zr1	C6	C7	C8	65.2(2)	C10	C6	C7	Zr1	-63.9(2)
C12	Zr1	C7	C6	105.0(2)	C11	Zr1	C7	C6	145.4(2)
C9	Zr1	C7	C6	78.2(2)	C8	Zr1	C7	C6	116.0(3)
C10	Zr1	C7	C6	36.8(2)	C1	Zr1	C7	C6	-8.6(3)
C2	Zr1	C7	C6	-31.0(2)	C3	Zr1	C7	C6	-63.0(2)
C4	Zr1	C7	C6	-76.6(3)	C5	Zr1	C7	C6	-32.5(3)
C12	Zr1	C7	C8	-11.1(2)	C11	Zr1	C7	C8	29.3(2)
C9	Zr1	C7	C8	-37.82(19)	C10	Zr1	C7	C8	-79.2(2)
C1	Zr1	C7	C8	-124.69(19)	C2	Zr1	C7	C8	-147.01(19)
C3	Zr1	C7	C8	-179.05(19)	C4	Zr1	C7	C8	167.33(18)
C5	Zr1	C7	C8	-148.5(2)	C6	Zr1	C7	C8	-116.0(3)
C6	C7	C8	C9	-0.2(3)	Zr1	C7	C8	C9	67.0(2)
C6	C7	C8	Zr1	-67.2(2)	C12	Zr1	C8	C7	170.82(19)
C11	Zr1	C8	C7	-155.56(19)	C9	Zr1	C8	C7	114.3(3)
C10	Zr1	C8	C7	75.9(2)	C1	Zr1	C8	C7	80.8(2)
C2	Zr1	C8	C7	40.8(2)	C3	Zr1	C8	C7	1.3(3)
C4	Zr1	C8	C7	-33.4(4)	C5	Zr1	C8	C7	114.0(4)
C6	Zr1	C8	C7	35.79(19)	C12	Zr1	C8	C9	56.5(2)
C11	Zr1	C8	C9	90.2(2)	C10	Zr1	C8	C9	-38.4(2)
C1	Zr1	C8	C9	-33.5(3)	C2	Zr1	C8	C9	-73.4(2)
C3	Zr1	C8	C9	-113.0(2)	C7	Zr1	C8	C9	-114.3(3)
C4	Zr1	C8	C9	-147.6(3)	C5	Zr1	C8	C9	-0.3(5)
C6	Zr1	C8	C9	-78.5(2)	C7	C8	C9	C10	-1.0(3)
Zr1	C8	C9	C10	67.5(2)	C7	C8	C9	Zr1	-68.5(2)
C12	Zr1	C9	C8	-120.6(2)	C11	Zr1	C9	C8	-92.16(19)
C10	Zr1	C9	C8	112.7(3)	C1	Zr1	C9	C8	156.41(19)
C2	Zr1	C9	C8	122.6(2)	C3	Zr1	C9	C8	103.2(2)
C7	Zr1	C9	C8	36.79(18)	C4	Zr1	C9	C8	153.3(3)
C5	Zr1	C9	C8	179.91(18)	C6	Zr1	C9	C8	75.9(2)
C12	Zr1	C9	C10	126.7(2)	C11	Zr1	C9	C10	155.1(2)
C8	Zr1	C9	C10	-112.7(3)	C1	Zr1	C9	C10	43.7(2)
C2	Zr1	C9	C10	9.8(2)	C3	Zr1	C9	C10	-9.5(3)
C7	Zr1	C9	C10	-76.0(2)	C4	Zr1	C9	C10	40.5(4)
C5	Zr1	C9	C10	67.2(2)	C6	Zr1	C9	C10	-36.9(2)
C7	C6	C10	C9	-2.0(4)	Zr1	C6	C10	C9	-67.1(2)
C7	C6	C10	Zr1	65.1(2)	C8	C9	C10	C6	1.8(4)
Zr1	C9	C10	C6	69.3(2)	C8	C9	C10	Zr1	-67.5(2)
C12	Zr1	C10	C6	-165.4(2)	C11	Zr1	C10	C6	-144.2(2)
C9	Zr1	C10	C6	-114.1(3)	C8	Zr1	C10	C6	-76.0(2)
C1	Zr1	C10	C6	107.4(2)	C2	Zr1	C10	C6	75.2(2)
C3	Zr1	C10	C6	59.3(2)	C7	Zr1	C10	C6	-35.97(19)
C4	Zr1	C10	C6	83.0(2)	C5	Zr1	C10	C6	114.7(2)
C12	Zr1	C10	C9	-51.3(2)	C11	Zr1	C10	C9	-30.0(2)
C8	Zr1	C10	C9	38.16(19)	C1	Zr1	C10	C9	-138.4(2)
C2	Zr1	C10	C9	-170.7(2)	C3	Zr1	C10	C9	173.46(19)
C7	Zr1	C10	C9	78.2(2)	C4	Zr1	C10	C9	-162.88(17)

C5	Zr1	C10	C9	-131.2(2)	C6	Zr1	C10	C9	114.1(3)
C9	Zr1	C11	C12	-56.42(19)	C8	Zr1	C11	C12	-88.94(19)
C10	Zr1	C11	C12	-40.7(2)	C1	Zr1	C11	C12	53.5(2)
C2	Zr1	C11	C12	70.7(2)	C3	Zr1	C11	C12	111.0(2)
C7	Zr1	C11	C12	-103.86(19)	C4	Zr1	C11	C12	105.27(19)
C5	Zr1	C11	C12	75.11(19)					
C6	Zr1	C11	C12	-73.2(3)					
C12	Zr1	C11	P2#1	163.3(5)	C9	Zr1	C11	P2#1	106.8(4)
C8	Zr1	C11	P2#1	74.3(4)	C10	Zr1	C11	P2#1	122.5(4)
C1	Zr1	C11	P2#1	-143.3(4)	C2	Zr1	C11	P2#1	-126.0(4)
C3	Zr1	C11	P2#1	-85.8(4)	C7	Zr1	C11	P2#1	59.4(4)
C4	Zr1	C11	P2#1	-91.5(4)	C5	Zr1	C11	P2#1	-121.6(4)
C6	Zr1	C11	P2#1	90.1(4)	P2#1	C11	C12	C13	6.3(6)
Zr1	C11	C12	C13	176.8(4)	P2#1	C11	C12	Zr1	-170.5(3)
C9	Zr1	C12	C11	120.8(2)	C8	Zr1	C12	C11	93.25(19)
C10	Zr1	C12	C11	146.55(19)	C1	Zr1	C12	C11	-130.56(19)
C2	Zr1	C12	C11	-133.33(19)	C3	Zr1	C12	C11	-96.4(2)
C7	Zr1	C12	C11	99.0(2)	C4	Zr1	C12	C11	-79.79(19)
C5	Zr1	C12	C11	-100.3(2)	C6	Zr1	C12	C11	137.11(19)
C11	Zr1	C12	C13	-176.8(4)	C9	Zr1	C12	C13	-56.0(3)
C8	Zr1	C12	C13	-83.5(3)	C10	Zr1	C12	C13	-30.3(3)
C1	Zr1	C12	C13	52.6(3)	C2	Zr1	C12	C13	49.9(4)
C3	Zr1	C12	C13	86.8(4)	C7	Zr1	C12	C13	-77.8(3)
C4	Zr1	C12	C13	103.4(3)	C5	Zr1	C12	C13	82.9(3)
C6	Zr1	C12	C13	-39.7(4)	C11	C12	C13	C14	-71.1(5)
Zr1	C12	C13	C14	103.8(4)	C11	C12	C13	C18	112.0(5)
Zr1	C12	C13	C18	-73.0(4)	C18	C13	C14	C15	-1.2(5)
C12	C13	C14	C15	-178.1(3)	C13	C14	C15	C16	0.0(5)
C14	C15	C16	C17	0.8(5)	C15	C16	C17	C18	-0.4(5)
C16	C17	C18	C13	-0.8(5)	C14	C13	C18	C17	1.5(5)
C12	C13	C18	C17	178.5(3)	C11#1	P2	C19	C20	162.3(2)
C22	P2	C19	C20	50.8(3)	Zr1	P2	C19	C20	-81.1(2)
C11#1	P2	C19	C21	33.1(2)	C22	P2	C19	C21	-78.4(2)
Zr1	P2	C19	C21	149.70(18)	C11#1	P2	C22	C24	165.2(2)
C19	P2	C22	C24	-83.2(2)	Zr1	P2	C22	C24	45.4(2)
C11#1	P2	C22	C23	-64.9(3)	C19	P2	C22	C23	46.7(3)
Zr1	P2	C22	C23	175.30(19)					

X-Ray Structural Data for 4:

Data Collection

A fragment of a red plate crystal of $C_{38}H_{36}NPZr$ having approximate dimensions of 0.05 x 0.25 x 0.24 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX[1] CCD area detectorwith graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 4633 centered reflections with I > 10σ in the range 4.57 < 2θ < 52.08^o corresponded to a primitive monoclinic cell with dimensions:

a = 10.0566(6) Å
b = 8.5559(5) Å β = 94.276(1)^o
c = 35.792(2) Å
V = 3071.1(3) Å^3

For Z = 4 and F.W. = 628.90, the calculated density is 1.36 g/cm^3. The systematic absences of:

h0l: h+l $\neq$ 2n
0k0: k $\neq$ 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -100 $\pm$ 1^{o}C. Frames corresponding to an arbitrary hemisphereof data were collected using ω scans of 0.3^{o}counted for a total of 10.0 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[2] to a maximum 2θ value of 52.8^o.The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorptionusing XPREP[3]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[4]. (Tmax = 1.00, Tmin = 0.88).

Structure Solution and Refinement

The structure was solved by direct methods[5] and expanded using Fourier techniques[6]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[7] was based on 4780 observed reflections ($I > 3.00\sigma(I)$) and 370 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.032$$

$$R_w = [(\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2)]^{1/2} = 0.037$$

The standard deviation of an observation of unit weight[8] was 1.41. The weighting scheme was based on counting statistics and included a factor (p = 0.030) to downweight the intense reflections. Plots of Σ w $(|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.42 and -0.22 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[9]. Anomalous dispersion effects were included in Fcalc[10]; the values for Δf' and Δf" were those of Creagh and McAuley[11]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[12]. All calculations were performed using the teXsan[13] crystallographic software package of Molecular Structure Corporation.

A. Crystal Data

Empirical Formula	$C_{38}H_{36}NPZr$
Formula Weight	628.90
Crystal Color, Habit	red, plate
Crystal Dimensions	0.05 X 0.25 X 0.24 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.0566(6)Å
	b = 8.5559(5) Å
	c = 35.792(2) Å
	β = 94.276(1)^o
	V = 3071.1(3) $Å^3$
Space Group	$P2_1/n$ (#14)

Z value	4
D_{calc}	1.360 g/cm^3
F_{000}	1304.00
μ(MoKα)	4.37 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker APEX CCD
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	10.0 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
$2\theta_{max}$	52.8^o
No. of Reflections Measured (R_{int} = 0.031)	Total: 17434 Unique: 6624
Corrections	Lorentz-polarization
Absorption (Tmax = 1.00 Tmin = 0.88)	

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0300
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4780
No. Variables	370
Reflection/Parameter Ratio	12.92
Residuals: R; Rw; Rall	0.032 ; 0.037; 0.048
Goodness of Fit Indicator	1.41
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.42 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.22 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Zr(1)	0.63115(2)	0.15359(3)	0.668823(6)	1.477(5)	
P(1)	0.34759(6)	-0.03996(7)	0.61209(2)	1.81(1)	
N(1)	0.8542(2)	0.2436(2)	0.65588(6)	2.08(5)	
C(1)	0.4273(3)	0.3256(3)	0.67398(8)	2.30(6)	
C(2)	0.5273(3)	0.3960(3)	0.69762(7)	2.18(5)	
C(3)	0.6247(3)	0.4531(3)	0.67536(7)	2.27(6)	
C(4)	0.5828(3)	0.4203(3)	0.63736(7)	2.25(6)	
C(5)	0.4601(3)	0.3451(3)	0.63682(7)	2.21(5)	
C(6)	0.7589(3)	0.0788(3)	0.73112(7)	2.60(6)	
C(7)	0.6276(3)	0.0953(3)	0.73971(7)	2.45(6)	
C(8)	0.5511(3)	-0.0215(3)	0.72075(7)	2.37(6)	
C(9)	0.6387(3)	-0.1142(3)	0.70131(7)	2.44(6)	
C(10)	0.7662(3)	-0.0512(3)	0.70708(7)	2.49(6)	
C(11)	0.5155(2)	0.0074(3)	0.62725(6)	1.62(5)	
C(12)	0.6347(2)	0.0210(3)	0.61484(6)	1.63(5)	
C(13)	0.6957(2)	-0.0262(3)	0.58013(6)	1.78(5)	
C(14)	0.7926(2)	-0.1449(3)	0.58082(7)	2.16(5)	
C(15)	0.8483(3)	-0.1866(3)	0.54776(8)	2.54(6)	
C(16)	0.8151(3)	-0.1113(3)	0.51412(7)	2.57(6)	
C(17)	0.7209(3)	0.0075(3)	0.51400(7)	2.65(6)	
C(18)	0.6603(3)	0.0499(3)	0.54599(7)	2.23(6)	
C(19)	0.8352(3)	-0.2274(4)	0.61676(8)	3.20(7)	
C(20)	0.8809(3)	-0.1546(4)	0.47875(8)	3.68(7)	
C(21)	0.5569(3)	0.1773(3)	0.54426(7)	3.23(7)	
C(22)	0.3431(3)	-0.2187(3)	0.58338(7)	1.95(5)	
C(23)	0.2182(3)	-0.2744(3)	0.57029(8)	2.97(7)	
C(24)	0.2060(3)	-0.4021(4)	0.54667(9)	3.58(7)	
C(25)	0.3185(3)	-0.4750(3)	0.53508(8)	3.04(7)	
C(26)	0.4426(3)	-0.4199(3)	0.54770(7)	2.52(6)	
C(27)	0.4548(3)	-0.2933(3)	0.57184(7)	2.16(5)	
C(28)	0.2829(2)	-0.1168(3)	0.65534(7)	1.82(5)	
C(29)	0.1952(3)	-0.0243(3)	0.67392(7)	2.37(6)	
C(30)	0.1519(3)	-0.0710(3)	0.70819(8)	2.81(6)	
C(31)	0.1952(3)	-0.2099(3)	0.72408(7)	2.76(6)	
C(32)	0.2801(3)	-0.3055(3)	0.70530(7)	2.43(6)	
C(33)	0.3224(2)	-0.2596(3)	0.67122(7)	2.01(5)	
C(34)	0.8986(3)	0.2388(3)	0.62144(7)	2.61(6)	
C(35)	1.0122(3)	0.3164(3)	0.61217(8)	3.00(7)	
C(36)	1.0843(3)	0.4034(3)	0.63843(8)	2.85(6)	

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C(37)	1.0410(3)	0.4074(3)	0.67410(8)	2.95(6)	
C(38)	0.9275(3)	0.3273(3)	0.68143(7)	2.59(6)	
C(100)	0.5244	0.3880	0.6642	0.2000	0.000
C(101)	0.6685	-0.0025	0.7200	0.2000	0.000
H(1)	0.3504	0.2737	0.6818	2.7569	
H(2)	0.5287	0.4032	0.7243	2.5780	
H(3)	0.7050	0.5044	0.6841	2.7356	
H(4)	0.6308	0.4451	0.6161	2.6888	
H(5)	0.4075	0.3121	0.6150	2.6965	
H(6)	0.8314	0.1433	0.7401	3.0694	
H(7)	0.5947	0.1729	0.7557	2.9250	
H(8)	0.4575	-0.0349	0.7211	2.8960	
H(9)	0.6152	-0.2044	0.6869	2.9862	
H(10)	0.8444	-0.0886	0.6967	2.9957	
H(11)	0.9108	-0.2700	0.5482	3.0415	
H(12)	0.6975	0.0614	0.4911	3.1406	
H(13)	0.8794	-0.3231	0.6119	3.8965	
H(14)	0.7584	-0.2517	0.6303	3.8965	
H(15)	0.8935	-0.1633	0.6323	3.8965	
H(16)	0.9270	-0.2525	0.4822	4.4582	
H(17)	0.9440	-0.0767	0.4730	4.4582	
H(18)	0.8159	-0.1647	0.4582	4.4582	
H(19)	0.5427	0.2192	0.5197	4.0182	
H(20)	0.5824	0.2603	0.5613	4.0182	
H(21)	0.4722	0.1370	0.5515	4.0182	
H(22)	0.1404	-0.2236	0.5774	3.4984	
H(23)	0.1203	-0.4386	0.5380	4.2972	
H(24)	0.3100	-0.5627	0.5189	3.6167	
H(25)	0.5202	-0.4700	0.5401	3.0217	
H(26)	0.5409	-0.2571	0.5805	2.5908	
H(27)	0.1647	0.0718	0.6631	2.8492	
H(28)	0.0921	-0.0071	0.7206	3.3642	
H(29)	0.1670	-0.2407	0.7477	3.2927	
H(30)	0.3085	-0.4024	0.7161	2.9387	
H(31)	0.3792	-0.3267	0.6585	2.4528	
H(32)	0.8495	0.1792	0.6027	3.1297	
H(33)	1.0403	0.3087	0.5875	3.6152	
H(34)	1.1603	0.4604	0.6326	3.4487	
H(35)	1.0894	0.4640	0.6934	3.4615	

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(36)	0.8996	0.3312	0.7061	3.0546	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr(1)	0.0210(1)	0.0186(1)	0.0165(1)	0.00013(10)	0.00120(8)	0.00009(9)
P(1)	0.0230(4)	0.0230(3)	0.0227(3)	-0.0012(3)	0.0005(3)	-0.0002(3)
N(1)	0.026(1)	0.026(1)	0.027(1)	-0.0009(9)	0.0035(9)	-0.0032(9)
C(1)	0.023(1)	0.025(1)	0.040(2)	0.006(1)	0.007(1)	0.001(1)
C(2)	0.034(2)	0.025(1)	0.024(1)	0.008(1)	0.004(1)	-0.004(1)
C(3)	0.031(2)	0.019(1)	0.036(2)	0.002(1)	-0.000(1)	-0.004(1)
C(4)	0.039(2)	0.020(1)	0.027(1)	0.006(1)	0.008(1)	0.005(1)
C(5)	0.033(1)	0.022(1)	0.028(1)	0.010(1)	-0.007(1)	-0.002(1)
C(6)	0.040(2)	0.036(2)	0.021(1)	-0.008(1)	-0.009(1)	0.007(1)
C(7)	0.049(2)	0.028(1)	0.017(1)	0.003(1)	0.004(1)	0.004(1)
C(8)	0.033(2)	0.033(1)	0.024(1)	-0.004(1)	0.001(1)	0.010(1)
C(9)	0.049(2)	0.021(1)	0.022(1)	0.000(1)	-0.004(1)	0.005(1)
C(10)	0.033(2)	0.036(2)	0.026(1)	0.012(1)	0.001(1)	0.010(1)
C(11)	0.027(1)	0.017(1)	0.017(1)	0.0021(10)	0.001(1)	0.0021(9)
C(12)	0.024(1)	0.017(1)	0.020(1)	0.0009(10)	0.000(1)	0.0024(10)
C(13)	0.024(1)	0.023(1)	0.021(1)	-0.006(1)	0.003(1)	-0.003(1)
C(14)	0.025(1)	0.032(1)	0.025(1)	-0.004(1)	0.002(1)	-0.003(1)
C(15)	0.025(1)	0.035(2)	0.037(2)	-0.001(1)	0.007(1)	-0.011(1)
C(16)	0.033(2)	0.039(2)	0.026(1)	-0.011(1)	0.009(1)	-0.012(1)
C(17)	0.046(2)	0.033(2)	0.022(1)	-0.008(1)	0.006(1)	-0.003(1)
C(18)	0.037(2)	0.024(1)	0.024(1)	-0.003(1)	0.003(1)	-0.003(1)
C(19)	0.041(2)	0.043(2)	0.038(2)	0.017(1)	0.003(1)	0.000(1)
C(20)	0.049(2)	0.057(2)	0.036(2)	-0.010(2)	0.018(1)	-0.014(2)
C(21)	0.062(2)	0.039(2)	0.022(1)	0.013(1)	0.004(1)	0.004(1)
C(22)	0.029(1)	0.025(1)	0.020(1)	-0.004(1)	0.001(1)	0.001(1)
C(23)	0.030(2)	0.040(2)	0.043(2)	-0.005(1)	0.003(1)	-0.011(1)
C(24)	0.035(2)	0.048(2)	0.052(2)	-0.012(1)	-0.001(1)	-0.018(2)
C(25)	0.052(2)	0.033(2)	0.030(1)	-0.009(1)	0.005(1)	-0.010(1)
C(26)	0.036(2)	0.028(1)	0.032(1)	0.002(1)	0.007(1)	-0.001(1)
C(27)	0.028(1)	0.025(1)	0.028(1)	-0.003(1)	-0.002(1)	0.001(1)
C(28)	0.020(1)	0.025(1)	0.024(1)	-0.0042(10)	0.002(1)	-0.0048(10)
C(29)	0.026(1)	0.031(1)	0.034(1)	0.001(1)	0.002(1)	-0.005(1)
C(30)	0.028(2)	0.044(2)	0.037(2)	-0.002(1)	0.013(1)	-0.010(1)
C(31)	0.034(2)	0.044(2)	0.028(1)	-0.011(1)	0.011(1)	-0.002(1)
C(32)	0.033(2)	0.030(1)	0.030(1)	-0.007(1)	0.004(1)	0.001(1)
C(33)	0.026(1)	0.026(1)	0.025(1)	-0.004(1)	0.005(1)	-0.004(1)
C(34)	0.032(2)	0.037(2)	0.031(1)	-0.006(1)	0.005(1)	-0.007(1)
C(35)	0.038(2)	0.042(2)	0.036(2)	-0.005(1)	0.014(1)	-0.002(1)
C(36)	0.023(2)	0.035(2)	0.051(2)	-0.007(1)	0.006(1)	0.003(1)
C(37)	0.031(2)	0.039(2)	0.042(2)	-0.008(1)	-0.002(1)	-0.005(1)
C(38)	0.033(2)	0.036(2)	0.029(1)	-0.005(1)	0.001(1)	-0.005(1)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Zr(1)	N(1)	2.449(2)	Zr(1)	C(1)	2.542(2)
Zr(1)	C(2)	2.572(2)	Zr(1)	C(3)	2.575(3)
Zr(1)	C(4)	2.575(2)	Zr(1)	C(5)	2.582(2)
Zr(1)	C(6)	2.570(3)	Zr(1)	C(7)	2.589(2)
Zr(1)	C(8)	2.563(2)	Zr(1)	C(9)	2.568(2)
Zr(1)	C(10)	2.552(3)	Zr(1)	C(11)	2.208(2)
Zr(1)	C(12)	2.243(2)	Zr(1)	C(100)	2.2750(2)
Zr(1)	C(101)	2.2753(2)	P(1)	C(11)	1.781(2)
P(1)	C(22)	1.841(3)	P(1)	C(28)	1.844(2)
N(1)	C(34)	1.342(3)	N(1)	C(38)	1.339(3)
C(1)	C(2)	1.401(4)	C(1)	C(5)	1.404(4)
C(1)	C(100)	1.188(3)	C(2)	C(3)	1.396(3)
C(2)	C(100)	1.196(2)	C(3)	C(4)	1.421(4)
C(3)	C(100)	1.195(3)	C(4)	C(5)	1.391(4)
C(4)	C(100)	1.195(2)	C(5)	C(100)	1.191(2)
C(6)	C(7)	1.385(4)	C(6)	C(10)	1.412(4)
C(6)	C(101)	1.189(3)	C(7)	C(8)	1.405(4)
C(7)	C(101)	1.188(3)	C(8)	C(9)	1.408(4)
C(8)	C(101)	1.194(3)	C(9)	C(10)	1.392(4)
C(9)	C(101)	1.192(3)	C(10)	C(101)	1.192(3)
C(11)	C(12)	1.314(3)	C(12)	C(13)	1.482(3)
C(13)	C(14)	1.406(3)	C(13)	C(18)	1.407(3)
C(14)	C(15)	1.393(3)	C(14)	C(19)	1.501(4)
C(15)	C(16)	1.384(4)	C(16)	C(17)	1.390(4)
C(16)	C(20)	1.518(4)	C(17)	C(18)	1.385(3)
C(18)	C(21)	1.504(4)	C(22)	C(23)	1.392(4)
C(22)	C(27)	1.382(4)	C(23)	C(24)	1.381(4)
C(24)	C(25)	1.382(4)	C(25)	C(26)	1.378(4)
C(26)	C(27)	1.385(4)	C(28)	C(29)	1.391(3)
C(28)	C(33)	1.392(3)	C(29)	C(30)	1.390(4)
C(30)	C(31)	1.374(4)	C(31)	C(32)	1.390(4)
C(32)	C(33)	1.378(3)	C(34)	C(35)	1.383(4)
C(35)	C(36)	1.364(4)	C(36)	C(37)	1.380(4)
C(37)	C(38)	1.372(4)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.95	C(2)	H(2)	0.95
C(3)	H(3)	0.95	C(4)	H(4)	0.96
C(5)	H(5)	0.95	C(6)	H(6)	0.95
C(7)	H(7)	0.95	C(8)	H(8)	0.95
C(9)	H(9)	0.95	C(10)	H(10)	0.95
C(15)	H(11)	0.95	C(17)	H(12)	0.95
C(19)	H(13)	0.95	C(19)	H(14)	0.96
C(19)	H(15)	0.95	C(20)	H(16)	0.96
C(20)	H(17)	0.95	C(20)	H(18)	0.95
C(21)	H(19)	0.95	C(21)	H(20)	0.96
C(21)	H(21)	0.97	C(23)	H(22)	0.95
C(24)	H(23)	0.95	C(25)	H(24)	0.95
C(26)	H(25)	0.95	C(27)	H(26)	0.95
C(29)	H(27)	0.95	C(30)	H(28)	0.95
C(31)	H(29)	0.95	C(32)	H(30)	0.95
C(33)	H(31)	0.95	C(34)	H(32)	0.95
C(35)	H(33)	0.95	C(36)	H(34)	0.94
C(37)	H(35)	0.95	C(38)	H(36)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Zr(1)	C(1)	125.93(7)	N(1)	Zr(1)	C(2)	103.12(8)
N(1)	Zr(1)	C(3)	74.56(7)	N(1)	Zr(1)	C(4)	77.54(8)
N(1)	Zr(1)	C(5)	107.82(8)	N(1)	Zr(1)	C(6)	80.61(8)
N(1)	Zr(1)	C(7)	109.02(8)	N(1)	Zr(1)	C(8)	131.52(8)
N(1)	Zr(1)	C(9)	111.71(8)	N(1)	Zr(1)	C(10)	81.90(8)
N(1)	Zr(1)	C(11)	119.66(8)	N(1)	Zr(1)	C(12)	85.55(8)
N(1)	Zr(1)	C(100)	98.22(5)	N(1)	Zr(1)	C(101)	103.79(5)
C(1)	Zr(1)	C(2)	31.80(8)	C(1)	Zr(1)	C(3)	52.48(8)
C(1)	Zr(1)	C(4)	52.52(8)	C(1)	Zr(1)	C(5)	31.80(8)
C(1)	Zr(1)	C(6)	115.78(9)	C(1)	Zr(1)	C(7)	88.29(9)
C(1)	Zr(1)	C(8)	89.26(8)	C(1)	Zr(1)	C(9)	118.72(9)
C(1)	Zr(1)	C(10)	139.34(8)	C(1)	Zr(1)	C(11)	89.42(8)
C(1)	Zr(1)	C(12)	114.84(9)	C(1)	Zr(1)	C(100)	27.86(6)
C(1)	Zr(1)	C(101)	111.54(6)	C(2)	Zr(1)	C(3)	31.47(8)
C(2)	Zr(1)	C(4)	52.52(8)	C(2)	Zr(1)	C(5)	52.33(8)
C(2)	Zr(1)	C(6)	92.56(9)	C(2)	Zr(1)	C(7)	74.14(8)
C(2)	Zr(1)	C(8)	91.25(8)	C(2)	Zr(1)	C(9)	122.50(8)
C(2)	Zr(1)	C(10)	123.67(8)	C(2)	Zr(1)	C(11)	121.19(8)
C(2)	Zr(1)	C(12)	141.81(8)	C(2)	Zr(1)	C(100)	27.72(6)
C(2)	Zr(1)	C(101)	101.44(6)	C(3)	Zr(1)	C(4)	32.05(8)
C(3)	Zr(1)	C(5)	52.26(8)	C(3)	Zr(1)	C(6)	100.57(9)
C(3)	Zr(1)	C(7)	95.75(8)	C(3)	Zr(1)	C(8)	120.29(8)
C(3)	Zr(1)	C(9)	147.89(8)	C(3)	Zr(1)	C(10)	130.59(9)
C(3)	Zr(1)	C(11)	127.56(8)	C(3)	Zr(1)	C(12)	125.71(8)
C(3)	Zr(1)	C(100)	27.65(6)	C(3)	Zr(1)	C(101)	120.99(6)
C(4)	Zr(1)	C(5)	31.29(8)	C(4)	Zr(1)	C(6)	131.76(9)
C(4)	Zr(1)	C(7)	125.68(8)	C(4)	Zr(1)	C(8)	140.87(8)
C(4)	Zr(1)	C(9)	170.75(9)	C(4)	Zr(1)	C(10)	156.74(9)
C(4)	Zr(1)	C(11)	97.73(8)	C(4)	Zr(1)	C(12)	94.93(8)
C(4)	Zr(1)	C(100)	27.65(5)	C(4)	Zr(1)	C(101)	152.46(6)
C(5)	Zr(1)	C(6)	144.74(9)	C(5)	Zr(1)	C(7)	119.98(8)
C(5)	Zr(1)	C(8)	117.24(8)	C(5)	Zr(1)	C(9)	139.78(9)
C(5)	Zr(1)	C(10)	169.87(8)	C(5)	Zr(1)	C(11)	76.13(8)
C(5)	Zr(1)	C(12)	89.52(8)	C(5)	Zr(1)	C(100)	27.48(5)
C(5)	Zr(1)	C(101)	142.60(6)	C(6)	Zr(1)	C(7)	31.15(8)
C(6)	Zr(1)	C(8)	52.34(8)	C(6)	Zr(1)	C(9)	52.33(8)
C(6)	Zr(1)	C(10)	31.99(9)	C(6)	Zr(1)	C(11)	130.38(8)
C(6)	Zr(1)	C(12)	125.63(9)	C(6)	Zr(1)	C(100)	119.03(7)
C(6)	Zr(1)	C(101)	27.56(6)	C(7)	Zr(1)	C(8)	31.64(8)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(7)	Zr(1)	C(9)	52.15(8)	C(7)	Zr(1)	C(10)	52.24(8)
C(7)	Zr(1)	C(11)	120.43(8)	C(7)	Zr(1)	C(12)	138.53(8)
C(7)	Zr(1)	C(100)	101.54(6)	C(7)	Zr(1)	C(101)	27.31(6)
C(8)	Zr(1)	C(9)	31.84(8)	C(8)	Zr(1)	C(10)	52.64(8)
C(8)	Zr(1)	C(11)	88.82(8)	C(8)	Zr(1)	C(12)	110.81(8)
C(8)	Zr(1)	C(100)	113.32(6)	C(8)	Zr(1)	C(101)	27.77(6)
C(9)	Zr(1)	C(10)	31.56(8)	C(9)	Zr(1)	C(11)	78.23(8)
C(9)	Zr(1)	C(12)	86.40(8)	C(9)	Zr(1)	C(100)	144.82(6)
C(9)	Zr(1)	C(101)	27.66(6)	C(10)	Zr(1)	C(11)	101.84(9)
C(10)	Zr(1)	C(12)	94.19(8)	C(10)	Zr(1)	C(100)	150.89(6)
C(10)	Zr(1)	C(101)	27.84(6)	C(11)	Zr(1)	C(12)	34.34(8)
C(11)	Zr(1)	C(100)	103.20(6)	C(11)	Zr(1)	C(101)	104.90(6)
C(12)	Zr(1)	C(100)	114.89(6)	C(12)	Zr(1)	C(101)	112.61(6)
C(100)	Zr(1)	C(101)	128.657(10)	C(11)	P(1)	C(22)	110.0(1)
C(11)	P(1)	C(28)	102.2(1)	C(22)	P(1)	C(28)	100.2(1)
Zr(1)	N(1)	C(34)	122.4(2)	Zr(1)	N(1)	C(38)	120.3(2)
C(34)	N(1)	C(38)	116.1(2)	Zr(1)	C(1)	C(2)	75.3(1)
Zr(1)	C(1)	C(5)	75.7(1)	Zr(1)	C(1)	C(100)	63.5(1)
C(2)	C(1)	C(5)	108.2(2)	C(2)	C(1)	C(100)	54.3(1)
C(5)	C(1)	C(100)	53.9(1)	Zr(1)	C(2)	C(1)	72.9(1)
Zr(1)	C(2)	C(3)	74.4(1)	Zr(1)	C(2)	C(100)	62.2(1)
C(1)	C(2)	C(3)	108.0(2)	C(1)	C(2)	C(100)	53.7(1)
C(3)	C(2)	C(100)	54.2(1)	Zr(1)	C(3)	C(2)	74.2(1)
Zr(1)	C(3)	C(4)	74.0(1)	Zr(1)	C(3)	C(100)	62.1(1)
C(2)	C(3)	C(4)	107.9(2)	C(2)	C(3)	C(100)	54.3(1)
C(4)	C(3)	C(100)	53.5(1)	Zr(1)	C(4)	C(3)	73.9(1)
Zr(1)	C(4)	C(5)	74.6(1)	Zr(1)	C(4)	C(100)	62.1(1)
C(3)	C(4)	C(5)	107.7(2)	C(3)	C(4)	C(100)	53.5(1)
C(5)	C(4)	C(100)	54.2(1)	Zr(1)	C(5)	C(1)	72.5(1)
Zr(1)	C(5)	C(4)	74.1(1)	Zr(1)	C(5)	C(100)	61.8(1)
C(1)	C(5)	C(4)	108.2(2)	C(1)	C(5)	C(100)	53.7(1)
C(4)	C(5)	C(100)	54.5(1)	Zr(1)	C(6)	C(7)	75.2(1)
Zr(1)	C(6)	C(10)	73.3(1)	Zr(1)	C(6)	C(101)	62.3(1)
C(7)	C(6)	C(10)	108.1(2)	C(7)	C(6)	C(101)	54.3(2)
C(10)	C(6)	C(101)	53.7(2)	Zr(1)	C(7)	C(6)	73.7(1)
Zr(1)	C(7)	C(8)	73.2(1)	Zr(1)	C(7)	C(101)	61.50(10)
C(6)	C(7)	C(8)	108.5(2)	C(6)	C(7)	C(101)	54.4(2)
C(8)	C(7)	C(101)	54.1(2)	Zr(1)	C(8)	C(7)	75.2(1)
Zr(1)	C(8)	C(9)	74.3(1)	Zr(1)	C(8)	C(101)	62.6(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(7)	C(8)	C(9)	107.4(2)	C(7)	C(8)	C(101)	53.7(2)
C(9)	C(8)	C(101)	53.8(2)	Zr(1)	C(9)	C(8)	73.9(1)
Zr(1)	C(9)	C(10)	73.6(1)	Zr(1)	C(9)	C(101)	62.4(1)
C(8)	C(9)	C(10)	108.2(2)	C(8)	C(9)	C(101)	53.9(2)
C(10)	C(9)	C(101)	54.3(2)	Zr(1)	C(10)	C(6)	74.7(1)
Zr(1)	C(10)	C(9)	74.8(1)	Zr(1)	C(10)	C(101)	63.1(1)
C(6)	C(10)	C(9)	107.8(2)	C(6)	C(10)	C(101)	53.5(2)
C(9)	C(10)	C(101)	54.3(2)	Zr(1)	C(11)	P(1)	140.7(1)
Zr(1)	C(11)	C(12)	74.3(1)	P(1)	C(11)	C(12)	141.7(2)
Zr(1)	C(12)	C(11)	71.4(1)	Zr(1)	C(12)	C(13)	153.4(2)
C(11)	C(12)	C(13)	134.7(2)	C(12)	C(13)	C(14)	120.8(2)
C(12)	C(13)	C(18)	120.5(2)	C(14)	C(13)	C(18)	118.7(2)
C(13)	C(14)	C(15)	119.5(2)	C(13)	C(14)	C(19)	120.5(2)
C(15)	C(14)	C(19)	120.0(2)	C(14)	C(15)	C(16)	122.2(2)
C(15)	C(16)	C(17)	117.6(2)	C(15)	C(16)	C(20)	121.4(3)
C(17)	C(16)	C(20)	121.0(3)	C(16)	C(17)	C(18)	122.1(2)
C(13)	C(18)	C(17)	119.9(2)	C(13)	C(18)	C(21)	120.1(2)
C(17)	C(18)	C(21)	120.1(2)	P(1)	C(22)	C(23)	117.2(2)
P(1)	C(22)	C(27)	124.3(2)	C(23)	C(22)	C(27)	118.3(2)
C(22)	C(23)	C(24)	120.9(3)	C(23)	C(24)	C(25)	120.2(3)
C(24)	C(25)	C(26)	119.3(3)	C(25)	C(26)	C(27)	120.5(2)
C(22)	C(27)	C(26)	120.8(2)	P(1)	C(28)	C(29)	118.3(2)
P(1)	C(28)	C(33)	123.2(2)	C(29)	C(28)	C(33)	118.4(2)
C(28)	C(29)	C(30)	120.6(2)	C(29)	C(30)	C(31)	120.2(2)
C(30)	C(31)	C(32)	119.7(2)	C(31)	C(32)	C(33)	120.1(2)
C(28)	C(33)	C(32)	120.9(2)	N(1)	C(34)	C(35)	122.9(2)
C(34)	C(35)	C(36)	120.1(3)	C(35)	C(36)	C(37)	117.6(2)
C(36)	C(37)	C(38)	119.3(3)	N(1)	C(38)	C(37)	124.0(2)
Zr(1)	C(100)	C(1)	88.7(1)	Zr(1)	C(100)	C(2)	90.1(1)
Zr(1)	C(100)	C(3)	90.3(1)	Zr(1)	C(100)	C(4)	90.3(1)
Zr(1)	C(100)	C(5)	90.7(1)	C(1)	C(100)	C(2)	72.0(2)
C(1)	C(100)	C(3)	143.4(2)	C(1)	C(100)	C(4)	143.6(2)
C(1)	C(100)	C(5)	72.3(2)	C(2)	C(100)	C(3)	71.4(2)
C(2)	C(100)	C(4)	144.4(2)	C(2)	C(100)	C(5)	144.3(2)
C(3)	C(100)	C(4)	73.0(2)	C(3)	C(100)	C(5)	144.3(2)
C(4)	C(100)	C(5)	71.3(2)	Zr(1)	C(101)	C(6)	90.1(1)
Zr(1)	C(101)	C(7)	91.2(1)	Zr(1)	C(101)	C(8)	89.6(1)
Zr(1)	C(101)	C(9)	90.0(1)	Zr(1)	C(101)	C(10)	89.1(1)
C(6)	C(101)	C(7)	71.3(2)	C(6)	C(101)	C(8)	143.5(2)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	C(101)	C(9)	144.2(2)	C(6)	C(101)	C(10)	72.7(2)
C(7)	C(101)	C(8)	72.3(2)	C(7)	C(101)	C(9)	144.5(2)
C(7)	C(101)	C(10)	144.0(2)	C(8)	C(101)	C(9)	72.3(2)
C(8)	C(101)	C(10)	143.7(2)	C(9)	C(101)	C(10)	71.5(2)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Zr(1)	C(1)	H(1)	115.4	C(2)	C(1)	H(1)	125.7
C(5)	C(1)	H(1)	126.1	C(100)	C(1)	H(1)	178.8
Zr(1)	C(2)	H(2)	118.4	C(1)	C(2)	H(2)	125.9
C(3)	C(2)	H(2)	126.1	C(100)	C(2)	H(2)	179.3
Zr(1)	C(3)	H(3)	117.6	C(2)	C(3)	H(3)	125.9
C(4)	C(3)	H(3)	126.2	C(100)	C(3)	H(3)	179.6
Zr(1)	C(4)	H(4)	117.1	C(3)	C(4)	H(4)	126.0
C(5)	C(4)	H(4)	126.3	C(100)	C(4)	H(4)	179.0
Zr(1)	C(5)	H(5)	119.1	C(1)	C(5)	H(5)	125.9
C(4)	C(5)	H(5)	125.9	C(100)	C(5)	H(5)	179.0
Zr(1)	C(6)	H(6)	118.0	C(7)	C(6)	H(6)	125.8
C(10)	C(6)	H(6)	126.1	C(101)	C(6)	H(6)	179.6
Zr(1)	C(7)	H(7)	119.0	C(6)	C(7)	H(7)	125.7
C(8)	C(7)	H(7)	125.8	C(101)	C(7)	H(7)	179.4
Zr(1)	C(8)	H(8)	116.5	C(7)	C(8)	H(8)	126.0
C(9)	C(8)	H(8)	126.6	C(101)	C(8)	H(8)	179.0
Zr(1)	C(9)	H(9)	118.8	C(8)	C(9)	H(9)	126.0
C(10)	C(9)	H(9)	125.8	C(101)	C(9)	H(9)	178.8
Zr(1)	C(10)	H(10)	116.3	C(6)	C(10)	H(10)	125.9
C(9)	C(10)	H(10)	126.3	C(101)	C(10)	H(10)	179.2
C(14)	C(15)	H(11)	119.0	C(16)	C(15)	H(11)	118.8
C(16)	C(17)	H(12)	118.7	C(18)	C(17)	H(12)	119.2
C(14)	C(19)	H(13)	110.7	C(14)	C(19)	H(14)	110.1
C(14)	C(19)	H(15)	110.7	H(13)	C(19)	H(14)	108.0
H(13)	C(19)	H(15)	109.0	H(14)	C(19)	H(15)	108.2
C(16)	C(20)	H(16)	110.0	C(16)	C(20)	H(17)	110.3
C(16)	C(20)	H(18)	110.6	H(16)	C(20)	H(17)	108.3
H(16)	C(20)	H(18)	108.5	H(17)	C(20)	H(18)	109.1
C(18)	C(21)	H(19)	111.6	C(18)	C(21)	H(20)	111.1
C(18)	C(21)	H(21)	110.4	H(19)	C(21)	H(20)	108.8
H(19)	C(21)	H(21)	107.8	H(20)	C(21)	H(21)	107.0
C(22)	C(23)	H(22)	119.7	C(24)	C(23)	H(22)	119.4
C(23)	C(24)	H(23)	119.8	C(25)	C(24)	H(23)	119.9
C(24)	C(25)	H(24)	120.1	C(26)	C(25)	H(24)	120.6
C(25)	C(26)	H(25)	119.8	C(27)	C(26)	H(25)	119.7
C(22)	C(27)	H(26)	119.5	C(26)	C(27)	H(26)	119.7
C(28)	C(29)	H(27)	119.6	C(30)	C(29)	H(27)	119.8
C(29)	C(30)	H(28)	119.9	C(31)	C(30)	H(28)	119.9
C(30)	C(31)	H(29)	120.1	C(32)	C(31)	H(29)	120.2

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(31)	C(32)	H(30)	119.6	C(33)	C(32)	H(30)	120.3
C(28)	C(33)	H(31)	119.8	C(32)	C(33)	H(31)	119.3
N(1)	C(34)	H(32)	118.2	C(35)	C(34)	H(32)	118.9
C(34)	C(35)	H(33)	119.9	C(36)	C(35)	H(33)	120.0
C(35)	C(36)	H(34)	121.8	C(37)	C(36)	H(34)	120.6
C(36)	C(37)	H(35)	120.4	C(38)	C(37)	H(35)	120.4
N(1)	C(38)	H(36)	118.0	C(37)	C(38)	H(36)	118.0

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Zr(1)	N(1)	C(34)	C(35)	166.8(2)	Zr(1)	N(1)	C(38)	C(37)	-166.9(2)
Zr(1)	C(1)	C(2)	C(3)	66.7(2)	Zr(1)	C(1)	C(2)	C(100)	67.68(9)
Zr(1)	C(1)	C(5)	C(4)	-66.1(2)	Zr(1)	C(1)	C(5)	C(100)	-67.43(9)
Zr(1)	C(1)	C(100)	C(2)	-90.5(1)	Zr(1)	C(1)	C(100)	C(3)	-88.6(3)
Zr(1)	C(1)	C(100)	C(4)	88.7(3)	Zr(1)	C(1)	C(100)	C(5)	91.2(1)
Zr(1)	C(2)	C(1)	C(5)	-69.2(2)	Zr(1)	C(2)	C(1)	C(100)	-67.68(9)
Zr(1)	C(2)	C(3)	C(4)	66.9(2)	Zr(1)	C(2)	C(3)	C(100)	66.71(9)
Zr(1)	C(2)	C(100)	C(1)	88.6(1)	Zr(1)	C(2)	C(100)	C(3)	-90.2(1)
Zr(1)	C(2)	C(100)	C(4)	-90.6(3)	Zr(1)	C(2)	C(100)	C(5)	91.4(2)
Zr(1)	C(3)	C(2)	C(1)	-65.7(2)	Zr(1)	C(3)	C(2)	C(100)	-66.71(9)
Zr(1)	C(3)	C(4)	C(5)	67.6(2)	Zr(1)	C(3)	C(4)	C(100)	66.82(9)
Zr(1)	C(3)	C(100)	C(1)	88.1(2)	Zr(1)	C(3)	C(100)	C(2)	90.0(1)
Zr(1)	C(3)	C(100)	C(4)	-90.2(1)	Zr(1)	C(3)	C(100)	C(5)	-91.6(3)
Zr(1)	C(4)	C(3)	C(2)	-67.0(2)	Zr(1)	C(4)	C(3)	C(100)	-66.82(9)
Zr(1)	C(4)	C(5)	C(1)	65.0(2)	Zr(1)	C(4)	C(5)	C(100)	66.39(9)
Zr(1)	C(4)	C(100)	C(1)	-88.1(2)	Zr(1)	C(4)	C(100)	C(2)	90.6(3)
Zr(1)	C(4)	C(100)	C(3)	90.2(1)	Zr(1)	C(4)	C(100)	C(5)	-90.7(1)
Zr(1)	C(5)	C(1)	C(2)	68.9(2)	Zr(1)	C(5)	C(1)	C(100)	67.43(9)
Zr(1)	C(5)	C(4)	C(3)	-67.1(2)	Zr(1)	C(5)	C(4)	C(100)	-66.39(9)
Zr(1)	C(5)	C(100)	C(1)	-88.4(1)	Zr(1)	C(5)	C(100)	C(2)	-91.2(2)
Zr(1)	C(5)	C(100)	C(3)	91.5(3)	Zr(1)	C(5)	C(100)	C(4)	90.1(1)
Zr(1)	C(6)	C(7)	C(8)	65.4(2)	Zr(1)	C(6)	C(7)	C(101)	66.31(9)
Zr(1)	C(6)	C(10)	C(9)	-68.1(2)	Zr(1)	C(6)	C(10)	C(101)	-67.55(10)
Zr(1)	C(6)	C(101)	C(7)	-91.2(1)	Zr(1)	C(6)	C(101)	C(8)	-89.6(3)
Zr(1)	C(6)	C(101)	C(9)	90.1(3)	Zr(1)	C(6)	C(101)	C(10)	89.0(1)
Zr(1)	C(7)	C(6)	C(10)	-66.5(2)	Zr(1)	C(7)	C(6)	C(101)	-66.31(9)
Zr(1)	C(7)	C(8)	C(9)	67.8(2)	Zr(1)	C(7)	C(8)	C(101)	66.63(9)
Zr(1)	C(7)	C(101)	C(6)	89.7(1)	Zr(1)	C(7)	C(101)	C(8)	-89.2(1)
Zr(1)	C(7)	C(101)	C(9)	-91.6(3)	Zr(1)	C(7)	C(101)	C(10)	90.1(3)
Zr(1)	C(8)	C(7)	C(6)	-65.8(2)	Zr(1)	C(8)	C(7)	C(101)	-66.63(9)
Zr(1)	C(8)	C(9)	C(10)	66.2(2)	Zr(1)	C(8)	C(9)	C(101)	67.26(9)
Zr(1)	C(8)	C(101)	C(6)	89.7(3)	Zr(1)	C(8)	C(101)	C(7)	91.4(1)
Zr(1)	C(8)	C(101)	C(9)	-90.1(1)	Zr(1)	C(8)	C(101)	C(10)	-88.0(3)
Zr(1)	C(9)	C(8)	C(7)	-68.5(2)	Zr(1)	C(9)	C(8)	C(101)	-67.26(9)
Zr(1)	C(9)	C(10)	C(6)	68.0(2)	Zr(1)	C(9)	C(10)	C(101)	67.45(10)
Zr(1)	C(9)	C(101)	C(6)	-90.2(3)	Zr(1)	C(9)	C(101)	C(7)	92.0(3)
Zr(1)	C(9)	C(101)	C(8)	89.6(1)	Zr(1)	C(9)	C(101)	C(10)	-89.1(1)
Zr(1)	C(10)	C(6)	C(7)	67.8(2)	Zr(1)	C(10)	C(6)	C(101)	67.55(10)
Zr(1)	C(10)	C(9)	C(8)	-66.4(2)	Zr(1)	C(10)	C(9)	C(101)	-67.45(10)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Zr(1)	C(10)	C(101)	C(6)	-90.4(1)	Zr(1)	C(10)	C(101)	C(7)	-90.8(3)
Zr(1)	C(10)	C(101)	C(8)	88.2(3)	Zr(1)	C(10)	C(101)	C(9)	90.3(1)
Zr(1)	C(11)	P(1)	C(22)	-163.9(2)	Zr(1)	C(11)	P(1)	C(28)	-58.2(2)
Zr(1)	C(11)	C(12)	C(13)	-173.8(3)	Zr(1)	C(12)	C(11)	P(1)	160.4(3)
Zr(1)	C(12)	C(13)	C(14)	82.2(4)	Zr(1)	C(12)	C(13)	C(18)	-96.1(4)
Zr(1)	C(100)	C(1)	C(2)	90.5(1)	Zr(1)	C(100)	C(1)	C(5)	-91.2(1)
Zr(1)	C(100)	C(2)	C(1)	-88.6(1)	Zr(1)	C(100)	C(2)	C(3)	90.2(1)
Zr(1)	C(100)	C(3)	C(2)	-90.0(1)	Zr(1)	C(100)	C(3)	C(4)	90.2(1)
Zr(1)	C(100)	C(4)	C(3)	-90.2(1)	Zr(1)	C(100)	C(4)	C(5)	90.7(1)
Zr(1)	C(100)	C(5)	C(1)	88.4(1)	Zr(1)	C(100)	C(5)	C(4)	-90.1(1)
Zr(1)	C(101)	C(6)	C(7)	91.2(1)	Zr(1)	C(101)	C(6)	C(10)	-89.0(1)
Zr(1)	C(101)	C(7)	C(6)	-89.7(1)	Zr(1)	C(101)	C(7)	C(8)	89.2(1)
Zr(1)	C(101)	C(8)	C(7)	-91.4(1)	Zr(1)	C(101)	C(8)	C(9)	90.1(1)
Zr(1)	C(101)	C(9)	C(8)	-89.6(1)	Zr(1)	C(101)	C(9)	C(10)	89.1(1)
Zr(1)	C(101)	C(10)	C(6)	90.4(1)	Zr(1)	C(101)	C(10)	C(9)	-90.3(1)
P(1)	C(11)	Zr(1)	N(1)	-153.4(2)	P(1)	C(11)	Zr(1)	C(1)	-21.4(2)
P(1)	C(11)	Zr(1)	C(2)	-22.8(2)	P(1)	C(11)	Zr(1)	C(3)	-60.5(2)
P(1)	C(11)	Zr(1)	C(4)	-73.4(2)	P(1)	C(11)	Zr(1)	C(5)	-50.6(2)
P(1)	C(11)	Zr(1)	C(6)	102.9(2)	P(1)	C(11)	Zr(1)	C(7)	66.3(2)
P(1)	C(11)	Zr(1)	C(8)	67.9(2)	P(1)	C(11)	Zr(1)	C(9)	98.2(2)
P(1)	C(11)	Zr(1)	C(10)	119.3(2)	P(1)	C(11)	Zr(1)	C(12)	-160.8(3)
P(1)	C(11)	Zr(1)	C(100)	-45.8(2)	P(1)	C(11)	Zr(1)	C(101)	90.8(2)
P(1)	C(11)	C(12)	C(13)	-13.5(5)	P(1)	C(22)	C(23)	C(24)	175.9(2)
P(1)	C(22)	C(27)	C(26)	-174.6(2)	P(1)	C(28)	C(29)	C(30)	-174.8(2)
P(1)	C(28)	C(33)	C(32)	174.2(2)	N(1)	Zr(1)	C(1)	C(2)	-50.5(2)
N(1)	Zr(1)	C(1)	C(5)	63.1(2)	N(1)	Zr(1)	C(1)	C(100)	6.6(2)
N(1)	Zr(1)	C(2)	C(1)	140.1(1)	N(1)	Zr(1)	C(2)	C(3)	25.2(2)
N(1)	Zr(1)	C(2)	C(100)	82.6(1)	N(1)	Zr(1)	C(3)	C(2)	-154.5(2)
N(1)	Zr(1)	C(3)	C(4)	91.1(2)	N(1)	Zr(1)	C(3)	C(100)	147.9(1)
N(1)	Zr(1)	C(4)	C(3)	-80.7(2)	N(1)	Zr(1)	C(4)	C(5)	165.2(2)
N(1)	Zr(1)	C(4)	C(100)	-137.5(1)	N(1)	Zr(1)	C(5)	C(1)	-130.6(1)
N(1)	Zr(1)	C(5)	C(4)	-15.2(2)	N(1)	Zr(1)	C(5)	C(100)	-73.0(1)
N(1)	Zr(1)	C(6)	C(7)	155.8(2)	N(1)	Zr(1)	C(6)	C(10)	-89.7(2)
N(1)	Zr(1)	C(6)	C(101)	-147.0(1)	N(1)	Zr(1)	C(7)	C(6)	-25.3(2)
N(1)	Zr(1)	C(7)	C(8)	-141.0(2)	N(1)	Zr(1)	C(7)	C(101)	-83.2(1)
N(1)	Zr(1)	C(8)	C(7)	52.6(2)	N(1)	Zr(1)	C(8)	C(9)	-60.7(2)
N(1)	Zr(1)	C(8)	C(101)	-3.8(2)	N(1)	Zr(1)	C(9)	C(8)	135.3(1)
N(1)	Zr(1)	C(9)	C(10)	20.3(2)	N(1)	Zr(1)	C(9)	C(101)	78.1(1)
N(1)	Zr(1)	C(10)	C(6)	85.2(2)	N(1)	Zr(1)	C(10)	C(9)	-161.0(2)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(1)	Zr(1)	C(10)	C(101)	141.7(1)	N(1)	Zr(1)	C(11)	C(12)	7.4(2)
N(1)	Zr(1)	C(12)	C(11)	-173.5(1)	N(1)	Zr(1)	C(12)	C(13)	-3.4(4)
N(1)	Zr(1)	C(100)	C(1)	-174.6(1)	N(1)	Zr(1)	C(100)	C(2)	-102.6(1)
N(1)	Zr(1)	C(100)	C(3)	-31.2(1)	N(1)	Zr(1)	C(100)	C(4)	41.8(1)
N(1)	Zr(1)	C(100)	C(5)	113.1(1)	N(1)	Zr(1)	C(101)	C(6)	33.6(1)
N(1)	Zr(1)	C(101)	C(7)	104.8(1)	N(1)	Zr(1)	C(101)	C(8)	177.1(1)
N(1)	Zr(1)	C(101)	C(9)	-110.6(1)	N(1)	Zr(1)	C(101)	C(10)	-39.1(1)
N(1)	C(34)	C(35)	C(36)	-0.4(5)	N(1)	C(38)	C(37)	C(36)	0.1(5)
C(1)	Zr(1)	N(1)	C(34)	-98.0(2)	C(1)	Zr(1)	N(1)	C(38)	69.1(2)
C(1)	Zr(1)	C(2)	C(3)	-114.9(2)	C(1)	Zr(1)	C(2)	C(100)	-57.5(1)
C(1)	Zr(1)	C(3)	C(2)	37.1(1)	C(1)	Zr(1)	C(3)	C(4)	-77.3(2)
C(1)	Zr(1)	C(3)	C(100)	-20.6(1)	C(1)	Zr(1)	C(4)	C(3)	77.2(2)
C(1)	Zr(1)	C(4)	C(5)	-36.8(1)	C(1)	Zr(1)	C(4)	C(100)	20.5(1)
C(1)	Zr(1)	C(5)	C(4)	115.5(2)	C(1)	Zr(1)	C(5)	C(100)	57.7(1)
C(1)	Zr(1)	C(6)	C(7)	30.3(2)	C(1)	Zr(1)	C(6)	C(10)	144.8(2)
C(1)	Zr(1)	C(6)	C(101)	87.5(1)	C(1)	Zr(1)	C(7)	C(6)	-152.9(2)
C(1)	Zr(1)	C(7)	C(8)	91.4(2)	C(1)	Zr(1)	C(7)	C(101)	149.1(1)
C(1)	Zr(1)	C(8)	C(7)	-87.9(2)	C(1)	Zr(1)	C(8)	C(9)	158.7(2)
C(1)	Zr(1)	C(8)	C(101)	-144.3(1)	C(1)	Zr(1)	C(9)	C(8)	-24.4(2)
C(1)	Zr(1)	C(9)	C(10)	-139.5(2)	C(1)	Zr(1)	C(9)	C(101)	-81.7(2)
C(1)	Zr(1)	C(10)	C(6)	-52.8(2)	C(1)	Zr(1)	C(10)	C(9)	60.9(2)
C(1)	Zr(1)	C(10)	C(101)	3.7(2)	C(1)	Zr(1)	C(11)	C(12)	139.4(1)
C(1)	Zr(1)	C(12)	C(11)	-45.8(2)	C(1)	Zr(1)	C(12)	C(13)	124.4(4)
C(1)	Zr(1)	C(100)	C(2)	72.0(2)	C(1)	Zr(1)	C(100)	C(3)	143.4(2)
C(1)	Zr(1)	C(100)	C(4)	-143.6(2)	C(1)	Zr(1)	C(100)	C(5)	-72.3(2)
C(1)	Zr(1)	C(101)	C(6)	-104.7(2)	C(1)	Zr(1)	C(101)	C(7)	-33.4(2)
C(1)	Zr(1)	C(101)	C(8)	38.8(1)	C(1)	Zr(1)	C(101)	C(9)	111.1(2)
C(1)	Zr(1)	C(101)	C(10)	-177.4(2)	C(1)	C(2)	Zr(1)	C(3)	114.9(2)
C(1)	C(2)	Zr(1)	C(4)	77.4(2)	C(1)	C(2)	Zr(1)	C(5)	37.6(1)
C(1)	C(2)	Zr(1)	C(6)	-138.9(2)	C(1)	C(2)	Zr(1)	C(7)	-113.5(2)
C(1)	C(2)	Zr(1)	C(8)	-86.6(2)	C(1)	C(2)	Zr(1)	C(9)	-93.1(2)
C(1)	C(2)	Zr(1)	C(10)	-130.9(2)	C(1)	C(2)	Zr(1)	C(11)	2.8(2)
C(1)	C(2)	Zr(1)	C(12)	40.5(2)	C(1)	C(2)	Zr(1)	C(100)	57.5(1)
C(1)	C(2)	Zr(1)	C(101)	-112.6(1)	C(1)	C(2)	C(3)	C(4)	1.2(3)
C(1)	C(2)	C(3)	C(100)	1.0(2)	C(1)	C(2)	C(100)	C(3)	-178.8(2)
C(1)	C(2)	C(100)	C(4)	-179.2(3)	C(1)	C(2)	C(100)	C(5)	2.8(3)
C(1)	C(5)	Zr(1)	C(2)	-37.6(1)	C(1)	C(5)	Zr(1)	C(3)	-77.7(2)
C(1)	C(5)	Zr(1)	C(4)	-115.5(2)	C(1)	C(5)	Zr(1)	C(6)	-31.6(2)
C(1)	C(5)	Zr(1)	C(7)	-5.1(2)	C(1)	C(5)	Zr(1)	C(8)	30.9(2)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	C(5)	Zr(1)	C(9)	60.3(2)	C(1)	C(5)	Zr(1)	C(10)	32.6(5)
C(1)	C(5)	Zr(1)	C(11)	112.2(2)	C(1)	C(5)	Zr(1)	C(12)	144.2(2)
C(1)	C(5)	Zr(1)	C(100)	-57.7(1)	C(1)	C(5)	Zr(1)	C(101)	15.7(2)
C(1)	C(5)	C(4)	C(3)	-2.1(3)	C(1)	C(5)	C(4)	C(100)	-1.4(2)
C(1)	C(5)	C(100)	C(2)	-2.8(3)	C(1)	C(5)	C(100)	C(3)	179.8(3)
C(1)	C(5)	C(100)	C(4)	178.4(2)	C(1)	C(100)	Zr(1)	C(2)	-72.0(2)
C(1)	C(100)	Zr(1)	C(3)	-143.4(2)	C(1)	C(100)	Zr(1)	C(4)	143.6(2)
C(1)	C(100)	Zr(1)	C(5)	72.3(2)	C(1)	C(100)	Zr(1)	C(6)	-90.8(1)
C(1)	C(100)	Zr(1)	C(7)	-63.2(1)	C(1)	C(100)	Zr(1)	C(8)	-32.3(1)
C(1)	C(100)	Zr(1)	C(9)	-26.0(2)	C(1)	C(100)	Zr(1)	C(10)	-86.5(2)
C(1)	C(100)	Zr(1)	C(11)	62.2(1)	C(1)	C(100)	Zr(1)	C(12)	96.5(1)
C(1)	C(100)	Zr(1)	C(101)	-59.5(1)	C(1)	C(100)	C(2)	C(3)	178.8(2)
C(1)	C(100)	C(3)	C(2)	-1.9(3)	C(1)	C(100)	C(3)	C(4)	178.3(3)
C(1)	C(100)	C(4)	C(3)	-178.3(3)	C(1)	C(100)	C(4)	C(5)	2.6(3)
C(1)	C(100)	C(5)	C(4)	-178.4(2)	C(2)	Zr(1)	N(1)	C(34)	-122.7(2)
C(2)	Zr(1)	N(1)	C(38)	44.4(2)	C(2)	Zr(1)	C(1)	C(5)	113.6(2)
C(2)	Zr(1)	C(1)	C(100)	57.1(1)	C(2)	Zr(1)	C(3)	C(4)	-114.4(2)
C(2)	Zr(1)	C(3)	C(100)	-57.6(1)	C(2)	Zr(1)	C(4)	C(3)	36.8(1)
C(2)	Zr(1)	C(4)	C(5)	-77.2(2)	C(2)	Zr(1)	C(4)	C(100)	-19.9(1)
C(2)	Zr(1)	C(5)	C(4)	77.9(2)	C(2)	Zr(1)	C(5)	C(100)	20.1(1)
C(2)	Zr(1)	C(6)	C(7)	52.9(2)	C(2)	Zr(1)	C(6)	C(10)	167.4(2)
C(2)	Zr(1)	C(6)	C(101)	110.1(1)	C(2)	Zr(1)	C(7)	C(6)	-124.0(2)
C(2)	Zr(1)	C(7)	C(8)	120.3(2)	C(2)	Zr(1)	C(7)	C(101)	178.1(2)
C(2)	Zr(1)	C(8)	C(7)	-56.2(2)	C(2)	Zr(1)	C(8)	C(9)	-169.5(2)
C(2)	Zr(1)	C(8)	C(101)	-112.6(1)	C(2)	Zr(1)	C(9)	C(8)	12.4(2)
C(2)	Zr(1)	C(9)	C(10)	-102.6(2)	C(2)	Zr(1)	C(9)	C(101)	-44.8(2)
C(2)	Zr(1)	C(10)	C(6)	-15.2(2)	C(2)	Zr(1)	C(10)	C(9)	98.6(2)
C(2)	Zr(1)	C(10)	C(101)	41.3(2)	C(2)	Zr(1)	C(11)	C(12)	138.0(1)
C(2)	Zr(1)	C(12)	C(11)	-67.9(2)	C(2)	Zr(1)	C(12)	C(13)	102.3(4)
C(2)	Zr(1)	C(100)	C(3)	71.4(2)	C(2)	Zr(1)	C(100)	C(4)	144.4(2)
C(2)	Zr(1)	C(100)	C(5)	-144.3(2)	C(2)	Zr(1)	C(101)	C(6)	-73.2(2)
C(2)	Zr(1)	C(101)	C(7)	-1.9(2)	C(2)	Zr(1)	C(101)	C(8)	70.3(1)
C(2)	Zr(1)	C(101)	C(9)	142.6(2)	C(2)	Zr(1)	C(101)	C(10)	-145.9(2)
C(2)	C(1)	Zr(1)	C(3)	-36.7(1)	C(2)	C(1)	Zr(1)	C(4)	-77.4(2)
C(2)	C(1)	Zr(1)	C(5)	-113.6(2)	C(2)	C(1)	Zr(1)	C(6)	46.8(2)
C(2)	C(1)	Zr(1)	C(7)	61.9(2)	C(2)	C(1)	Zr(1)	C(8)	93.6(2)
C(2)	C(1)	Zr(1)	C(9)	106.2(2)	C(2)	C(1)	Zr(1)	C(10)	74.8(2)
C(2)	C(1)	Zr(1)	C(11)	-177.6(2)	C(2)	C(1)	Zr(1)	C(12)	-153.8(1)
C(2)	C(1)	Zr(1)	C(100)	-57.1(1)	C(2)	C(1)	Zr(1)	C(101)	76.6(1)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(2)	C(1)	C(5)	C(4)	2.8(3)	C(2)	C(1)	C(5)	C(100)	1.5(2)
C(2)	C(1)	C(100)	C(3)	1.9(3)	C(2)	C(1)	C(100)	C(4)	179.2(3)
C(2)	C(1)	C(100)	C(5)	-178.3(2)	C(2)	C(3)	Zr(1)	C(4)	114.4(2)
C(2)	C(3)	Zr(1)	C(5)	77.5(2)	C(2)	C(3)	Zr(1)	C(6)	-77.4(2)
C(2)	C(3)	Zr(1)	C(7)	-46.3(2)	C(2)	C(3)	Zr(1)	C(8)	-25.1(2)
C(2)	C(3)	Zr(1)	C(9)	-48.1(2)	C(2)	C(3)	Zr(1)	C(10)	-89.9(2)
C(2)	C(3)	Zr(1)	C(11)	89.7(2)	C(2)	C(3)	Zr(1)	C(12)	132.8(2)
C(2)	C(3)	Zr(1)	C(100)	57.6(1)	C(2)	C(3)	Zr(1)	C(101)	-57.5(2)
C(2)	C(3)	C(4)	C(5)	0.5(3)	C(2)	C(3)	C(4)	C(100)	-0.2(2)
C(2)	C(3)	C(100)	C(4)	179.8(2)	C(2)	C(3)	C(100)	C(5)	178.4(3)
C(2)	C(100)	Zr(1)	C(3)	-71.4(2)	C(2)	C(100)	Zr(1)	C(4)	-144.4(2)
C(2)	C(100)	Zr(1)	C(5)	144.3(2)	C(2)	C(100)	Zr(1)	C(6)	-18.8(1)
C(2)	C(100)	Zr(1)	C(7)	8.8(1)	C(2)	C(100)	Zr(1)	C(8)	39.7(1)
C(2)	C(100)	Zr(1)	C(9)	46.0(2)	C(2)	C(100)	Zr(1)	C(10)	-14.5(2)
C(2)	C(100)	Zr(1)	C(11)	134.2(1)	C(2)	C(100)	Zr(1)	C(12)	168.5(1)
C(2)	C(100)	Zr(1)	C(101)	12.5(1)	C(2)	C(100)	C(1)	C(5)	178.3(2)
C(2)	C(100)	C(3)	C(4)	-179.8(2)	C(2)	C(100)	C(4)	C(3)	0.4(3)
C(2)	C(100)	C(4)	C(5)	-178.8(3)	C(2)	C(100)	C(5)	C(4)	178.8(3)
C(3)	Zr(1)	N(1)	C(34)	-109.3(2)	C(3)	Zr(1)	N(1)	C(38)	57.8(2)
C(3)	Zr(1)	C(1)	C(5)	76.9(2)	C(3)	Zr(1)	C(1)	C(100)	20.4(1)
C(3)	Zr(1)	C(2)	C(100)	57.4(1)	C(3)	Zr(1)	C(4)	C(5)	-114.0(2)
C(3)	Zr(1)	C(4)	C(100)	-56.7(1)	C(3)	Zr(1)	C(5)	C(4)	37.8(1)
C(3)	Zr(1)	C(5)	C(100)	-20.0(1)	C(3)	Zr(1)	C(6)	C(7)	83.6(2)
C(3)	Zr(1)	C(6)	C(10)	-161.9(2)	C(3)	Zr(1)	C(6)	C(101)	140.8(1)
C(3)	Zr(1)	C(7)	C(6)	-100.9(2)	C(3)	Zr(1)	C(7)	C(8)	143.4(2)
C(3)	Zr(1)	C(7)	C(101)	-158.8(1)	C(3)	Zr(1)	C(8)	C(7)	-43.4(2)
C(3)	Zr(1)	C(8)	C(9)	-156.7(1)	C(3)	Zr(1)	C(8)	C(101)	-99.8(1)
C(3)	Zr(1)	C(9)	C(8)	39.9(2)	C(3)	Zr(1)	C(9)	C(10)	-75.2(2)
C(3)	Zr(1)	C(9)	C(101)	-17.4(2)	C(3)	Zr(1)	C(10)	C(6)	23.7(2)
C(3)	Zr(1)	C(10)	C(9)	137.4(2)	C(3)	Zr(1)	C(10)	C(101)	80.2(2)
C(3)	Zr(1)	C(11)	C(12)	100.3(2)	C(3)	Zr(1)	C(12)	C(11)	-106.2(1)
C(3)	Zr(1)	C(12)	C(13)	64.0(4)	C(3)	Zr(1)	C(100)	C(4)	73.0(2)
C(3)	Zr(1)	C(100)	C(5)	144.3(2)	C(3)	Zr(1)	C(101)	C(6)	-46.5(2)
C(3)	Zr(1)	C(101)	C(7)	24.8(2)	C(3)	Zr(1)	C(101)	C(8)	97.0(1)
C(3)	Zr(1)	C(101)	C(9)	169.3(2)	C(3)	Zr(1)	C(101)	C(10)	-119.2(2)
C(3)	C(2)	Zr(1)	C(4)	-37.5(1)	C(3)	C(2)	Zr(1)	C(5)	-77.3(2)
C(3)	C(2)	Zr(1)	C(6)	106.2(2)	C(3)	C(2)	Zr(1)	C(7)	131.6(2)
C(3)	C(2)	Zr(1)	C(8)	158.5(2)	C(3)	C(2)	Zr(1)	C(9)	152.0(1)
C(3)	C(2)	Zr(1)	C(10)	114.2(2)	C(3)	C(2)	Zr(1)	C(11)	-112.1(2)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(3)	C(2)	Zr(1)	C(12)	-74.4(2)	C(3)	C(2)	Zr(1)	C(100)	-57.4(1)
C(3)	C(2)	Zr(1)	C(101)	132.5(1)	C(3)	C(2)	C(1)	C(5)	-2.5(3)
C(3)	C(2)	C(1)	C(100)	-1.0(2)	C(3)	C(2)	C(100)	C(4)	-0.4(3)
C(3)	C(2)	C(100)	C(5)	-178.4(3)	C(3)	C(4)	Zr(1)	C(5)	114.0(2)
C(3)	C(4)	Zr(1)	C(6)	-15.7(2)	C(3)	C(4)	Zr(1)	C(7)	23.9(2)
C(3)	C(4)	Zr(1)	C(8)	62.8(2)	C(3)	C(4)	Zr(1)	C(9)	97.0(5)
C(3)	C(4)	Zr(1)	C(10)	-52.3(3)	C(3)	C(4)	Zr(1)	C(11)	160.5(2)
C(3)	C(4)	Zr(1)	C(12)	-165.1(2)	C(3)	C(4)	Zr(1)	C(100)	56.7(1)
C(3)	C(4)	Zr(1)	C(101)	15.2(2)	C(3)	C(4)	C(5)	C(100)	-0.7(2)
C(3)	C(4)	C(100)	C(5)	179.1(2)	C(3)	C(100)	Zr(1)	C(4)	-73.0(2)
C(3)	C(100)	Zr(1)	C(5)	-144.3(2)	C(3)	C(100)	Zr(1)	C(6)	52.6(1)
C(3)	C(100)	Zr(1)	C(7)	80.3(1)	C(3)	C(100)	Zr(1)	C(8)	111.1(1)
C(3)	C(100)	Zr(1)	C(9)	117.4(2)	C(3)	C(100)	Zr(1)	C(10)	56.9(2)
C(3)	C(100)	Zr(1)	C(11)	-154.4(1)	C(3)	C(100)	Zr(1)	C(12)	-120.1(1)
C(3)	C(100)	Zr(1)	C(101)	83.9(1)	C(3)	C(100)	C(1)	C(5)	-179.8(3)
C(3)	C(100)	C(4)	C(5)	-179.1(2)	C(3)	C(100)	C(5)	C(4)	1.4(3)
C(4)	Zr(1)	N(1)	C(34)	-76.4(2)	C(4)	Zr(1)	N(1)	C(38)	90.7(2)
C(4)	Zr(1)	C(1)	C(5)	36.2(1)	C(4)	Zr(1)	C(1)	C(100)	-20.3(1)
C(4)	Zr(1)	C(2)	C(100)	19.9(1)	C(4)	Zr(1)	C(3)	C(100)	56.8(1)
C(4)	Zr(1)	C(5)	C(100)	-57.8(1)	C(4)	Zr(1)	C(6)	C(7)	92.0(2)
C(4)	Zr(1)	C(6)	C(10)	-153.6(1)	C(4)	Zr(1)	C(6)	C(101)	149.1(1)
C(4)	Zr(1)	C(7)	C(6)	-113.4(2)	C(4)	Zr(1)	C(7)	C(8)	130.9(2)
C(4)	Zr(1)	C(7)	C(101)	-171.3(1)	C(4)	Zr(1)	C(8)	C(7)	-76.5(2)
C(4)	Zr(1)	C(8)	C(9)	170.1(1)	C(4)	Zr(1)	C(8)	C(101)	-132.9(1)
C(4)	Zr(1)	C(9)	C(8)	-42.3(6)	C(4)	Zr(1)	C(9)	C(10)	-157.4(5)
C(4)	Zr(1)	C(9)	C(101)	-99.6(5)	C(4)	Zr(1)	C(10)	C(6)	57.3(3)
C(4)	Zr(1)	C(10)	C(9)	171.0(2)	C(4)	Zr(1)	C(10)	C(101)	113.8(2)
C(4)	Zr(1)	C(11)	C(12)	87.4(1)	C(4)	Zr(1)	C(12)	C(11)	-96.5(1)
C(4)	Zr(1)	C(12)	C(13)	73.7(4)	C(4)	Zr(1)	C(100)	C(5)	71.3(2)
C(4)	Zr(1)	C(101)	C(6)	-55.9(2)	C(4)	Zr(1)	C(101)	C(7)	15.4(2)
C(4)	Zr(1)	C(101)	C(8)	87.7(2)	C(4)	Zr(1)	C(101)	C(9)	160.0(2)
C(4)	Zr(1)	C(101)	C(10)	-128.6(2)	C(4)	C(3)	Zr(1)	C(5)	-36.9(1)
C(4)	C(3)	Zr(1)	C(6)	168.2(2)	C(4)	C(3)	Zr(1)	C(7)	-160.7(2)
C(4)	C(3)	Zr(1)	C(8)	-139.5(1)	C(4)	C(3)	Zr(1)	C(9)	-162.5(2)
C(4)	C(3)	Zr(1)	C(10)	155.7(1)	C(4)	C(3)	Zr(1)	C(11)	-24.7(2)
C(4)	C(3)	Zr(1)	C(12)	18.4(2)	C(4)	C(3)	Zr(1)	C(100)	-56.8(1)
C(4)	C(3)	Zr(1)	C(101)	-171.8(1)	C(4)	C(3)	C(2)	C(100)	0.2(2)
C(4)	C(3)	C(100)	C(5)	-1.4(3)	C(4)	C(5)	Zr(1)	C(6)	83.9(2)
C(4)	C(5)	Zr(1)	C(7)	110.3(2)	C(4)	C(5)	Zr(1)	C(8)	146.4(1)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(4)	C(5)	Zr(1)	C(9)	175.8(1)	C(4)	C(5)	Zr(1)	C(10)	148.1(4)
C(4)	C(5)	Zr(1)	C(11)	-132.3(2)	C(4)	C(5)	Zr(1)	C(12)	-100.3(2)
C(4)	C(5)	Zr(1)	C(100)	57.8(1)	C(4)	C(5)	Zr(1)	C(101)	131.2(1)
C(4)	C(5)	C(1)	C(100)	1.4(2)	C(4)	C(100)	Zr(1)	C(5)	-71.3(2)
C(4)	C(100)	Zr(1)	C(6)	125.6(2)	C(4)	C(100)	Zr(1)	C(7)	153.3(1)
C(4)	C(100)	Zr(1)	C(8)	-175.9(1)	C(4)	C(100)	Zr(1)	C(9)	-169.6(2)
C(4)	C(100)	Zr(1)	C(10)	129.9(2)	C(4)	C(100)	Zr(1)	C(11)	-81.4(1)
C(4)	C(100)	Zr(1)	C(12)	-47.1(1)	C(4)	C(100)	Zr(1)	C(101)	156.9(1)
C(4)	C(100)	C(1)	C(5)	-2.5(3)	C(5)	Zr(1)	N(1)	C(34)	-68.4(2)
C(5)	Zr(1)	N(1)	C(38)	98.7(2)	C(5)	Zr(1)	C(1)	C(100)	-56.5(1)
C(5)	Zr(1)	C(2)	C(100)	-19.9(1)	C(5)	Zr(1)	C(3)	C(100)	19.9(1)
C(5)	Zr(1)	C(4)	C(100)	57.3(1)	C(5)	Zr(1)	C(6)	C(7)	48.2(2)
C(5)	Zr(1)	C(6)	C(10)	162.6(2)	C(5)	Zr(1)	C(6)	C(101)	105.3(2)
C(5)	Zr(1)	C(7)	C(6)	-150.2(2)	C(5)	Zr(1)	C(7)	C(8)	94.1(2)
C(5)	Zr(1)	C(7)	C(101)	151.9(1)	C(5)	Zr(1)	C(8)	C(7)	-103.6(2)
C(5)	Zr(1)	C(8)	C(9)	143.0(1)	C(5)	Zr(1)	C(8)	C(101)	-160.0(1)
C(5)	Zr(1)	C(9)	C(8)	-55.9(2)	C(5)	Zr(1)	C(9)	C(10)	-171.0(1)
C(5)	Zr(1)	C(9)	C(101)	-113.2(1)	C(5)	Zr(1)	C(10)	C(6)	-78.7(5)
C(5)	Zr(1)	C(10)	C(9)	35.1(5)	C(5)	Zr(1)	C(10)	C(101)	-22.2(6)
C(5)	Zr(1)	C(11)	C(12)	110.2(1)	C(5)	Zr(1)	C(12)	C(11)	-65.6(1)
C(5)	Zr(1)	C(12)	C(13)	104.6(4)	C(5)	Zr(1)	C(101)	C(6)	-113.6(2)
C(5)	Zr(1)	C(101)	C(7)	-42.3(2)	C(5)	Zr(1)	C(101)	C(8)	30.0(2)
C(5)	Zr(1)	C(101)	C(9)	102.3(2)	C(5)	Zr(1)	C(101)	C(10)	173.7(2)
C(5)	C(1)	Zr(1)	C(6)	160.4(1)	C(5)	C(1)	Zr(1)	C(7)	175.5(2)
C(5)	C(1)	Zr(1)	C(8)	-152.8(2)	C(5)	C(1)	Zr(1)	C(9)	-140.2(1)
C(5)	C(1)	Zr(1)	C(10)	-171.6(2)	C(5)	C(1)	Zr(1)	C(11)	-64.0(2)
C(5)	C(1)	Zr(1)	C(12)	-40.2(2)	C(5)	C(1)	Zr(1)	C(100)	56.5(1)
C(5)	C(1)	Zr(1)	C(101)	-169.8(1)	C(5)	C(1)	C(2)	C(100)	-1.5(2)
C(5)	C(4)	Zr(1)	C(6)	-129.7(2)	C(5)	C(4)	Zr(1)	C(7)	-90.2(2)
C(5)	C(4)	Zr(1)	C(8)	-51.3(2)	C(5)	C(4)	Zr(1)	C(9)	-17.0(6)
C(5)	C(4)	Zr(1)	C(10)	-166.4(2)	C(5)	C(4)	Zr(1)	C(11)	46.4(2)
C(5)	C(4)	Zr(1)	C(12)	80.9(2)	C(5)	C(4)	Zr(1)	C(100)	-57.3(1)
C(5)	C(4)	Zr(1)	C(101)	-98.8(2)	C(5)	C(4)	C(3)	C(100)	0.7(2)
C(5)	C(100)	Zr(1)	C(6)	-163.1(1)	C(5)	C(100)	Zr(1)	C(7)	-135.4(1)
C(5)	C(100)	Zr(1)	C(8)	-104.6(1)	C(5)	C(100)	Zr(1)	C(9)	-98.3(2)
C(5)	C(100)	Zr(1)	C(10)	-158.8(2)	C(5)	C(100)	Zr(1)	C(11)	-10.1(1)
C(5)	C(100)	Zr(1)	C(12)	24.2(1)	C(5)	C(100)	Zr(1)	C(101)	-131.8(1)
C(6)	Zr(1)	N(1)	C(34)	146.9(2)	C(6)	Zr(1)	N(1)	C(38)	-46.0(2)
C(6)	Zr(1)	C(1)	C(100)	103.9(1)	C(6)	Zr(1)	C(2)	C(100)	163.6(1)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(6)	Zr(1)	C(3)	C(100)	-135.0(1)	C(6)	Zr(1)	C(4)	C(100)	-72.4(2)
C(6)	Zr(1)	C(5)	C(100)	26.1(2)	C(6)	Zr(1)	C(7)	C(8)	-115.7(2)
C(6)	Zr(1)	C(7)	C(101)	-57.9(2)	C(6)	Zr(1)	C(8)	C(7)	36.1(2)
C(6)	Zr(1)	C(8)	C(9)	-77.3(2)	C(6)	Zr(1)	C(8)	C(101)	-20.3(1)
C(6)	Zr(1)	C(9)	C(8)	77.3(2)	C(6)	Zr(1)	C(9)	C(10)	-37.8(1)
C(6)	Zr(1)	C(9)	C(101)	20.0(1)	C(6)	Zr(1)	C(10)	C(9)	113.7(2)
C(6)	Zr(1)	C(10)	C(101)	56.5(2)	C(6)	Zr(1)	C(11)	C(12)	-96.4(2)
C(6)	Zr(1)	C(12)	C(11)	111.3(1)	C(6)	Zr(1)	C(12)	C(13)	-78.5(4)
C(6)	Zr(1)	C(101)	C(7)	71.3(2)	C(6)	Zr(1)	C(101)	C(8)	143.5(2)
C(6)	Zr(1)	C(101)	C(9)	-144.2(2)	C(6)	Zr(1)	C(101)	C(10)	-72.7(2)
C(6)	C(7)	Zr(1)	C(8)	115.7(2)	C(6)	C(7)	Zr(1)	C(9)	77.8(2)
C(6)	C(7)	Zr(1)	C(10)	37.6(2)	C(6)	C(7)	Zr(1)	C(11)	118.7(2)
C(6)	C(7)	Zr(1)	C(12)	80.1(2)	C(6)	C(7)	Zr(1)	C(100)	-128.3(2)
C(6)	C(7)	Zr(1)	C(101)	57.9(2)	C(6)	C(7)	C(8)	C(9)	2.1(3)
C(6)	C(7)	C(8)	C(101)	0.9(2)	C(6)	C(7)	C(101)	C(8)	-179.0(2)
C(6)	C(7)	C(101)	C(9)	178.7(3)	C(6)	C(7)	C(101)	C(10)	0.4(3)
C(6)	C(10)	Zr(1)	C(7)	-36.6(1)	C(6)	C(10)	Zr(1)	C(8)	-76.8(2)
C(6)	C(10)	Zr(1)	C(9)	-113.7(2)	C(6)	C(10)	Zr(1)	C(11)	-156.0(2)
C(6)	C(10)	Zr(1)	C(12)	170.1(2)	C(6)	C(10)	Zr(1)	C(100)	-7.1(2)
C(6)	C(10)	Zr(1)	C(101)	-56.5(2)	C(6)	C(10)	C(9)	C(8)	1.7(3)
C(6)	C(10)	C(9)	C(101)	0.6(2)	C(6)	C(10)	C(101)	C(7)	-0.4(3)
C(6)	C(10)	C(101)	C(8)	178.6(3)	C(6)	C(10)	C(101)	C(9)	-179.3(2)
C(6)	C(101)	Zr(1)	C(7)	-71.3(2)	C(6)	C(101)	Zr(1)	C(8)	-143.5(2)
C(6)	C(101)	Zr(1)	C(9)	144.2(2)	C(6)	C(101)	Zr(1)	C(10)	72.7(2)
C(6)	C(101)	Zr(1)	C(11)	159.9(2)	C(6)	C(101)	Zr(1)	C(12)	124.5(2)
C(6)	C(101)	Zr(1)	C(100)	-79.1(1)	C(6)	C(101)	C(7)	C(8)	179.0(2)
C(6)	C(101)	C(8)	C(7)	-1.6(3)	C(6)	C(101)	C(8)	C(9)	179.8(3)
C(6)	C(101)	C(9)	C(8)	-179.8(3)	C(6)	C(101)	C(9)	C(10)	-1.1(3)
C(6)	C(101)	C(10)	C(9)	179.3(2)	C(7)	Zr(1)	N(1)	C(34)	159.8(2)
C(7)	Zr(1)	N(1)	C(38)	-33.1(2)	C(7)	Zr(1)	C(1)	C(100)	119.0(1)
C(7)	Zr(1)	C(2)	C(100)	-171.0(1)	C(7)	Zr(1)	C(3)	C(100)	-103.9(1)
C(7)	Zr(1)	C(4)	C(100)	-32.9(2)	C(7)	Zr(1)	C(5)	C(100)	52.5(2)
C(7)	Zr(1)	C(6)	C(10)	114.5(2)	C(7)	Zr(1)	C(6)	C(101)	57.1(2)
C(7)	Zr(1)	C(8)	C(9)	-113.3(2)	C(7)	Zr(1)	C(8)	C(101)	-56.4(2)
C(7)	Zr(1)	C(9)	C(8)	37.6(1)	C(7)	Zr(1)	C(9)	C(10)	-77.5(2)
C(7)	Zr(1)	C(9)	C(101)	-19.7(1)	C(7)	Zr(1)	C(10)	C(9)	77.2(2)
C(7)	Zr(1)	C(10)	C(101)	19.9(1)	C(7)	Zr(1)	C(11)	C(12)	-132.9(1)
C(7)	Zr(1)	C(12)	C(11)	72.5(2)	C(7)	Zr(1)	C(12)	C(13)	-117.3(4)
C(7)	Zr(1)	C(101)	C(8)	72.2(2)	C(7)	Zr(1)	C(101)	C(9)	144.5(2)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(7)	Zr(1)	C(101)	C(10)	-144.0(2)	C(7)	C(6)	Zr(1)	C(8)	-36.7(2)
C(7)	C(6)	Zr(1)	C(9)	-77.2(2)	C(7)	C(6)	Zr(1)	C(10)	-114.5(2)
C(7)	C(6)	Zr(1)	C(11)	-83.0(2)	C(7)	C(6)	Zr(1)	C(12)	-126.6(2)
C(7)	C(6)	Zr(1)	C(100)	61.6(2)	C(7)	C(6)	Zr(1)	C(101)	-57.1(2)
C(7)	C(6)	C(10)	C(9)	-0.4(3)	C(7)	C(6)	C(10)	C(101)	0.2(2)
C(7)	C(6)	C(101)	C(8)	1.6(3)	C(7)	C(6)	C(101)	C(9)	-178.7(3)
C(7)	C(6)	C(101)	C(10)	-179.8(2)	C(7)	C(8)	Zr(1)	C(9)	113.3(2)
C(7)	C(8)	Zr(1)	C(10)	76.7(2)	C(7)	C(8)	Zr(1)	C(11)	-177.4(2)
C(7)	C(8)	Zr(1)	C(12)	155.7(2)	C(7)	C(8)	Zr(1)	C(100)	-73.5(2)
C(7)	C(8)	Zr(1)	C(101)	56.4(2)	C(7)	C(8)	C(9)	C(10)	-2.3(3)
C(7)	C(8)	C(9)	C(101)	-1.2(2)	C(7)	C(8)	C(101)	C(9)	178.6(2)
C(7)	C(8)	C(101)	C(10)	-179.4(3)	C(7)	C(101)	Zr(1)	C(8)	-72.2(2)
C(7)	C(101)	Zr(1)	C(9)	-144.5(2)	C(7)	C(101)	Zr(1)	C(10)	144.0(2)
C(7)	C(101)	Zr(1)	C(11)	-128.8(2)	C(7)	C(101)	Zr(1)	C(12)	-164.3(2)
C(7)	C(101)	Zr(1)	C(100)	-7.8(1)	C(7)	C(101)	C(6)	C(10)	179.8(2)
C(7)	C(101)	C(8)	C(9)	-178.6(2)	C(7)	C(101)	C(9)	C(8)	2.4(3)
C(7)	C(101)	C(9)	C(10)	-178.9(3)	C(7)	C(101)	C(10)	C(9)	179.0(3)
C(8)	Zr(1)	N(1)	C(34)	133.7(2)	C(8)	Zr(1)	N(1)	C(38)	-59.2(2)
C(8)	Zr(1)	C(1)	C(100)	150.6(1)	C(8)	Zr(1)	C(2)	C(100)	-144.1(1)
C(8)	Zr(1)	C(3)	C(100)	-82.7(1)	C(8)	Zr(1)	C(4)	C(100)	6.0(2)
C(8)	Zr(1)	C(5)	C(100)	88.6(1)	C(8)	Zr(1)	C(6)	C(10)	77.8(2)
C(8)	Zr(1)	C(6)	C(101)	20.5(1)	C(8)	Zr(1)	C(7)	C(101)	57.8(2)
C(8)	Zr(1)	C(9)	C(10)	-115.1(2)	C(8)	Zr(1)	C(9)	C(101)	-57.3(1)
C(8)	Zr(1)	C(10)	C(9)	37.0(1)	C(8)	Zr(1)	C(10)	C(101)	-20.3(1)
C(8)	Zr(1)	C(11)	C(12)	-131.3(1)	C(8)	Zr(1)	C(12)	C(11)	53.5(2)
C(8)	Zr(1)	C(12)	C(13)	-136.3(4)	C(8)	Zr(1)	C(101)	C(9)	72.3(2)
C(8)	Zr(1)	C(101)	C(10)	143.8(2)	C(8)	C(7)	Zr(1)	C(9)	-37.8(2)
C(8)	C(7)	Zr(1)	C(10)	-78.1(2)	C(8)	C(7)	Zr(1)	C(11)	3.1(2)
C(8)	C(7)	Zr(1)	C(12)	-35.6(2)	C(8)	C(7)	Zr(1)	C(100)	116.0(2)
C(8)	C(7)	Zr(1)	C(101)	-57.8(2)	C(8)	C(7)	C(6)	C(10)	-1.1(3)
C(8)	C(7)	C(6)	C(101)	-0.9(2)	C(8)	C(7)	C(101)	C(9)	-2.4(3)
C(8)	C(7)	C(101)	C(10)	179.4(3)	C(8)	C(9)	Zr(1)	C(10)	115.1(2)
C(8)	C(9)	Zr(1)	C(11)	-107.2(2)	C(8)	C(9)	Zr(1)	C(12)	-140.9(2)
C(8)	C(9)	Zr(1)	C(100)	-10.9(2)	C(8)	C(9)	Zr(1)	C(101)	57.3(1)
C(8)	C(9)	C(10)	C(101)	1.1(2)	C(8)	C(9)	C(101)	C(10)	-178.7(2)
C(8)	C(101)	Zr(1)	C(9)	-72.3(2)	C(8)	C(101)	Zr(1)	C(10)	-143.8(2)
C(8)	C(101)	Zr(1)	C(11)	-56.6(1)	C(8)	C(101)	Zr(1)	C(12)	-92.0(1)
C(8)	C(101)	Zr(1)	C(100)	64.5(1)	C(8)	C(101)	C(6)	C(10)	-178.6(3)
C(8)	C(101)	C(9)	C(10)	178.7(2)	C(8)	C(101)	C(10)	C(9)	-2.1(3)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(9)	Zr(1)	N(1)	C(34)	104.0(2)	C(9)	Zr(1)	N(1)	C(38)	-88.9(2)
C(9)	Zr(1)	C(1)	C(100)	163.2(1)	C(9)	Zr(1)	C(2)	C(100)	-150.6(1)
C(9)	Zr(1)	C(3)	C(100)	-105.8(2)	C(9)	Zr(1)	C(4)	C(100)	40.3(6)
C(9)	Zr(1)	C(5)	C(100)	118.0(1)	C(9)	Zr(1)	C(6)	C(10)	37.2(1)
C(9)	Zr(1)	C(6)	C(101)	-20.1(1)	C(9)	Zr(1)	C(7)	C(101)	19.9(1)
C(9)	Zr(1)	C(8)	C(101)	56.9(2)	C(9)	Zr(1)	C(10)	C(101)	-57.2(1)
C(9)	Zr(1)	C(11)	C(12)	-101.0(1)	C(9)	Zr(1)	C(12)	C(11)	74.3(1)
C(9)	Zr(1)	C(12)	C(13)	-115.5(4)	C(9)	Zr(1)	C(101)	C(10)	71.5(2)
C(9)	C(8)	Zr(1)	C(10)	-36.6(1)	C(9)	C(8)	Zr(1)	C(11)	69.3(2)
C(9)	C(8)	Zr(1)	C(12)	42.3(2)	C(9)	C(8)	Zr(1)	C(100)	173.2(1)
C(9)	C(8)	Zr(1)	C(101)	-56.9(2)	C(9)	C(8)	C(7)	C(101)	1.2(2)
C(9)	C(8)	C(101)	C(10)	2.1(3)	C(9)	C(10)	Zr(1)	C(11)	-42.3(2)
C(9)	C(10)	Zr(1)	C(12)	-76.1(2)	C(9)	C(10)	Zr(1)	C(100)	106.6(2)
C(9)	C(10)	Zr(1)	C(101)	57.2(1)	C(9)	C(10)	C(6)	C(101)	-0.6(2)
C(9)	C(101)	Zr(1)	C(10)	-71.5(2)	C(9)	C(101)	Zr(1)	C(11)	15.7(2)
C(9)	C(101)	Zr(1)	C(12)	-19.7(2)	C(9)	C(101)	Zr(1)	C(100)	136.8(1)
C(9)	C(101)	C(6)	C(10)	1.1(3)	C(10)	Zr(1)	N(1)	C(34)	114.5(2)
C(10)	Zr(1)	N(1)	C(38)	-78.4(2)	C(10)	Zr(1)	C(1)	C(100)	131.8(1)
C(10)	Zr(1)	C(2)	C(100)	171.6(1)	C(10)	Zr(1)	C(3)	C(100)	-147.5(1)
C(10)	Zr(1)	C(4)	C(100)	-109.1(2)	C(10)	Zr(1)	C(5)	C(100)	90.3(5)
C(10)	Zr(1)	C(6)	C(101)	-57.3(2)	C(10)	Zr(1)	C(7)	C(101)	-20.3(1)
C(10)	Zr(1)	C(8)	C(101)	20.3(1)	C(10)	Zr(1)	C(9)	C(101)	57.8(2)
C(10)	Zr(1)	C(11)	C(12)	-79.9(1)	C(10)	Zr(1)	C(12)	C(11)	104.9(1)
C(10)	Zr(1)	C(12)	C(13)	-84.9(4)	C(10)	C(6)	Zr(1)	C(11)	31.5(2)
C(10)	C(6)	Zr(1)	C(12)	-12.1(2)	C(10)	C(6)	Zr(1)	C(100)	176.0(1)
C(10)	C(6)	Zr(1)	C(101)	57.3(2)	C(10)	C(6)	C(7)	C(101)	-0.2(2)
C(10)	C(9)	Zr(1)	C(11)	137.7(2)	C(10)	C(9)	Zr(1)	C(12)	104.0(2)
C(10)	C(9)	Zr(1)	C(100)	-126.0(1)	C(10)	C(9)	Zr(1)	C(101)	-57.8(2)
C(10)	C(9)	C(8)	C(101)	-1.1(2)	C(10)	C(101)	Zr(1)	C(11)	87.2(2)
C(10)	C(101)	Zr(1)	C(12)	51.7(2)	C(10)	C(101)	Zr(1)	C(100)	-151.8(1)
C(11)	Zr(1)	N(1)	C(34)	15.5(2)	C(11)	Zr(1)	N(1)	C(38)	-177.4(2)
C(11)	Zr(1)	C(1)	C(100)	-120.5(1)	C(11)	Zr(1)	C(2)	C(100)	-54.7(2)
C(11)	Zr(1)	C(3)	C(100)	32.1(2)	C(11)	Zr(1)	C(4)	C(100)	103.7(1)
C(11)	Zr(1)	C(5)	C(100)	169.9(1)	C(11)	Zr(1)	C(6)	C(101)	-25.9(2)
C(11)	Zr(1)	C(7)	C(101)	60.8(2)	C(11)	Zr(1)	C(8)	C(101)	126.2(1)
C(11)	Zr(1)	C(9)	C(101)	-164.5(2)	C(11)	Zr(1)	C(10)	C(101)	-99.5(1)
C(11)	Zr(1)	C(12)	C(13)	170.2(5)	C(11)	P(1)	C(22)	C(23)	178.0(2)
C(11)	P(1)	C(22)	C(27)	-7.0(3)	C(11)	P(1)	C(28)	C(29)	106.6(2)
C(11)	P(1)	C(28)	C(33)	-70.3(2)	C(11)	C(12)	Zr(1)	C(100)	-76.5(1)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(11)	C(12)	Zr(1)	C(101)	83.4(1)	C(11)	C(12)	C(13)	C(14)	-110.9(3)
C(11)	C(12)	C(13)	C(18)	70.8(4)	C(12)	Zr(1)	N(1)	C(34)	19.6(2)
C(12)	Zr(1)	N(1)	C(38)	-173.3(2)	C(12)	Zr(1)	C(1)	C(100)	-96.7(1)
C(12)	Zr(1)	C(2)	C(100)	-17.0(2)	C(12)	Zr(1)	C(3)	C(100)	75.2(1)
C(12)	Zr(1)	C(4)	C(100)	138.2(1)	C(12)	Zr(1)	C(5)	C(100)	-158.1(1)
C(12)	Zr(1)	C(6)	C(101)	-69.5(2)	C(12)	Zr(1)	C(7)	C(101)	22.2(2)
C(12)	Zr(1)	C(8)	C(101)	99.3(1)	C(12)	Zr(1)	C(9)	C(101)	161.8(1)
C(12)	Zr(1)	C(10)	C(101)	-133.4(1)	C(12)	C(11)	Zr(1)	C(100)	115.0(1)
C(12)	C(11)	Zr(1)	C(101)	-108.4(1)	C(12)	C(11)	P(1)	C(22)	46.8(3)
C(12)	C(11)	P(1)	C(28)	152.5(3)	C(12)	C(13)	C(14)	C(15)	-179.9(2)
C(12)	C(13)	C(14)	C(19)	0.7(4)	C(12)	C(13)	C(18)	C(17)	178.2(2)
C(12)	C(13)	C(18)	C(21)	-1.7(4)	C(13)	C(12)	Zr(1)	C(100)	93.6(4)
C(13)	C(12)	Zr(1)	C(101)	-106.5(4)	C(13)	C(14)	C(15)	C(16)	2.3(4)
C(13)	C(18)	C(17)	C(16)	1.3(4)	C(14)	C(13)	C(18)	C(17)	-0.1(4)
C(14)	C(13)	C(18)	C(21)	180.0(2)	C(14)	C(15)	C(16)	C(17)	-1.2(4)
C(14)	C(15)	C(16)	C(20)	177.7(2)	C(15)	C(14)	C(13)	C(18)	-1.6(4)
C(15)	C(16)	C(17)	C(18)	-0.6(4)	C(16)	C(15)	C(14)	C(19)	-178.2(2)
C(16)	C(17)	C(18)	C(21)	-178.8(3)	C(18)	C(13)	C(14)	C(19)	179.0(2)
C(18)	C(17)	C(16)	C(20)	-179.5(2)	C(22)	P(1)	C(28)	C(29)	-140.2(2)
C(22)	P(1)	C(28)	C(33)	42.9(2)	C(22)	C(23)	C(24)	C(25)	-1.2(5)
C(22)	C(27)	C(26)	C(25)	-0.8(4)	C(23)	C(22)	P(1)	C(28)	70.9(2)
C(23)	C(22)	C(27)	C(26)	0.3(4)	C(23)	C(24)	C(25)	C(26)	0.7(5)
C(24)	C(23)	C(22)	C(27)	0.7(4)	C(24)	C(25)	C(26)	C(27)	0.2(4)
C(27)	C(22)	P(1)	C(28)	-114.1(2)	C(28)	C(29)	C(30)	C(31)	-0.2(4)
C(28)	C(33)	C(32)	C(31)	0.9(4)	C(29)	C(28)	C(33)	C(32)	-2.6(4)
C(29)	C(30)	C(31)	C(32)	-1.5(4)	C(30)	C(29)	C(28)	C(33)	2.3(4)
C(30)	C(31)	C(32)	C(33)	1.2(4)	C(34)	N(1)	Zr(1)	C(100)	-94.9(2)
C(34)	N(1)	Zr(1)	C(101)	131.9(2)	C(34)	N(1)	C(38)	C(37)	0.9(4)
C(34)	C(35)	C(36)	C(37)	1.4(4)	C(35)	C(34)	N(1)	C(38)	-0.8(4)
C(35)	C(36)	C(37)	C(38)	-1.2(4)	C(38)	N(1)	Zr(1)	C(100)	72.2(2)
C(38)	N(1)	Zr(1)	C(101)	-61.1(2)	C(100)	Zr(1)	C(6)	C(101)	118.7(1)
C(100)	Zr(1)	C(7)	C(101)	173.8(1)	C(100)	Zr(1)	C(8)	C(101)	-129.9(1)
C(100)	Zr(1)	C(9)	C(101)	-68.2(2)	C(100)	Zr(1)	C(10)	C(101)	49.4(2)
C(100)	C(1)	Zr(1)	C(101)	133.7(1)	C(100)	C(2)	Zr(1)	C(101)	-170.1(1)
C(100)	C(3)	Zr(1)	C(101)	-115.08(10)	C(100)	C(4)	Zr(1)	C(101)	-41.5(2)
C(100)	C(5)	Zr(1)	C(101)	73.4(2)					

Table 8. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
C(2)	C(6)	3.572(4)	65602	C(2)	C(32)	3.589(4)	56501
C(4)	C(27)	3.565(4)	56501	C(32)	C(37)	3.559(4)	44501

X-Ray Structural Data for 5:

Data Collection

A fragment of a red block-like crystal of C50 H40 P2 Zr having approximate dimensions of 0.29 x 0.21 x 0.14 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a CCD area detector [10] CCD area detector with graphite monochromated MoKradiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 5505 centered reflections with I > 10σ(I) in the range $2.16 < \theta < 26.32^{o}$ corresponded to a primitive Monoclinic cell with dimensions:

a = 12.501(1) Å	$\alpha = 90^{o}$
b = 18.878(1) Å	$\beta = 108.181(1)^{o}$
c = 17.158(1) Å	$\gamma = 90^{o}$
V = 8876(1) Å^3	

For Z = 4 and F.W. = 793.98, the calculated density is 1.371 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

P2(1)/c

The data were collected at a temperature of 173(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3^{o} counted for a total of 30 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[11] to a maximum θ value of 26.40^{o}. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 1.00, Tmin = 0.84). Of the 22105 reflections that were collected, 7829 were unique (R_{int} = 0.0294); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined.

The final cycle of full-matrix least-squares refinement[3] was based on 7829 reflections (all data) and 478 variable parameters and converged (largest parameter shift was 0.001 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0377 \text{ for 6001 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.1107$$

The standard deviation of an observation of unit weight[4] was 0.868. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.540 and -0.861 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[9] crystallographic software package of Bruker Analytical X-ray Systems Inc.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C50 H40 P2 Zr
Formula Weight	793.98
Crystal Color, Habit	red, block
Crystal Dimensions	0.29 x 0.21 x 0.14 mm
Crystal System	Monoclinic
Lattice Type	primitive
Lattice Parameters	a = 12.501(1) Å b = 18.878(1) Å c = 17.158(1) Å α= 90 ° β= 108.181(1) ° γ = 90° V = 3847.1(3) $Å^3$
Space Group	P2(1)/c
Z value	4
D_{calc}	1.371 g/cm^3
F_{000}	1640

μ(MoK)	0.40 cm^{-1}

B. Intensity Measurements

Diffractometer	CCD area detector
Radiation	MoK(λ = 0.71073 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	30 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
θ_{max}	26.40^{o}
No. of Reflections Measured	Total: 22105 Unique: 7829 (R_{int} = 0.0294)
Corrections	Lorentz-polarization Absorption (Tmax = 1.00, Tmin = 0.84)

C. Structure Solution and Refinement

Structure Solution	direct (SHELXS-97 (Sheldrick, 1990))
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|F_o\|^2 - \|F_c\|^2)^2$
Least Squares Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (qP)^2 + 0.000P]$ where $P = [F_o^2 + 2F_c^2]/3$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	6001
No. Variables	478
Residuals: R; wR_2; Rall	0.0377; 0.1107; 0.0541
Goodness of Fit Indicator	0.868
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.540 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.861 $e^-/Å^3$

Table 1. Atomic coordinates and U_{iso}/U_{eq} and occupancy

atom	x	y	z	U_{eq}	Occupancy
Zr1	0.5076(1)	0.3020(1)	0.5134(1)	0.030(1)	1
P1	0.1839(1)	0.2749(1)	0.4473(1)	0.029(1)	1
P2	0.6781(1)	0.1982(1)	0.5604(1)	0.027(1)	1
C1	0.8478(2)	0.1955(2)	0.4881(2)	0.036(1)	1
C2	0.7400(2)	0.1709(1)	0.4822(1)	0.028(1)	1
C3	0.5584(2)	0.0360(1)	0.5928(1)	0.028(1)	1
C4	0.5928(2)	-0.0218(2)	0.6428(2)	0.037(1)	1
C5	0.3434(2)	0.1826(1)	0.5285(1)	0.025(1)	1
C6	0.1443(2)	0.2360(1)	0.3439(2)	0.030(1)	1
C7	0.3316(2)	0.2473(1)	0.4910(1)	0.025(1)	1
C8	0.5329(2)	0.1848(1)	0.5252(1)	0.026(1)	1
C9	0.2238(2)	0.0728(1)	0.5144(2)	0.031(1)	1
C10	0.8312(2)	0.0944(2)	0.6485(2)	0.037(1)	1
C11	0.2511(2)	0.1407(1)	0.5459(1)	0.027(1)	1
C12	0.7589(2)	0.1489(1)	0.6524(1)	0.030(1)	1
C13	0.1190(2)	0.1264(2)	0.6222(2)	0.036(1)	1
C14	0.4567(2)	0.0799(2)	0.6795(1)	0.033(1)	1
C15	0.1969(2)	0.1673(1)	0.6002(2)	0.032(1)	1
C16	0.1455(2)	0.0321(2)	0.5368(2)	0.036(1)	1
C17	0.4201(3)	0.3209(2)	0.3615(2)	0.045(1)	1
C18	0.2092(2)	0.1862(2)	0.3200(2)	0.041(1)	1
C19	0.5191(3)	0.3038(2)	0.6641(2)	0.054(1)	1
C20	0.6835(2)	0.1285(1)	0.4171(1)	0.032(1)	1
C21	0.5161(3)	0.2787(2)	0.3700(2)	0.055(1)	1
C22	0.8386(2)	0.1361(2)	0.3627(2)	0.044(1)	1
C23	-0.0020(2)	0.2175(2)	0.2150(2)	0.046(1)	1
C24	0.4583(2)	0.1505(1)	0.5540(1)	0.025(1)	1
C25	0.0371(2)	0.2506(1)	0.2897(2)	0.038(1)	1
C26	0.1807(2)	0.3709(1)	0.4266(2)	0.037(1)	1
C27	0.1780(2)	0.4022(2)	0.3523(2)	0.042(1)	1
C28	0.1677(2)	0.4758(2)	0.3425(2)	0.056(1)	1
C29	0.4895(2)	0.0877(1)	0.6094(1)	0.025(1)	1
C30	0.4232(2)	0.3443(2)	0.6231(2)	0.045(1)	1
C31	0.0943(2)	0.0588(2)	0.5912(2)	0.039(1)	1
C32	0.4579(3)	0.4056(2)	0.5910(2)	0.061(1)	1
C33	0.7429(2)	0.1622(2)	0.7274(2)	0.050(1)	1
C34	0.5595(2)	-0.0292(2)	0.7124(2)	0.040(1)	1
C35	0.4550(2)	0.3874(2)	0.3969(2)	0.054(1)	1
C36	0.7320(2)	0.1114(2)	0.3564(2)	0.040(1)	1
C37	0.8852(2)	0.0550(2)	0.7165(2)	0.044(1)	1

C38	0.6106(3)	0.3201(2)	0.4105(2)	0.069(1)	1
C39	0.0639(3)	0.1682(2)	0.1915(2)	0.048(1)	1
C40	0.6140(3)	0.3413(2)	0.6586(2)	0.073(1)	1
C41	0.1598(3)	0.4882(2)	0.4781(3)	0.065(1)	1
C42	0.1689(2)	0.4153(2)	0.4884(2)	0.048(1)	1
C43	0.4923(2)	0.0220(2)	0.7304(2)	0.039(1)	1
C44	0.5745(3)	0.3859(2)	0.4264(3)	0.075(1)	1
C45	0.8970(2)	0.1773(2)	0.4285(2)	0.043(1)	1
C46	0.1604(3)	0.5184(2)	0.4053(3)	0.071(1)	1
C47	0.1689(3)	0.1528(2)	0.2437(2)	0.049(1)	1
C48	0.8694(2)	0.0685(2)	0.7911(2)	0.051(1)	1
C49	0.5776(3)	0.4028(2)	0.6140(3)	0.074(1)	1
C50	0.7973(3)	0.1227(2)	0.7958(2)	0.062(1)	1

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr1	0.024(1)	0.025(1)	0.039(1)	-0.002(1)	0.008(1)	-0.004(1)
P1	0.023(1)	0.030(1)	0.034(1)	0.001(1)	0.007(1)	0.000(1)
P2	0.023(1)	0.031(1)	0.029(1)	0.000(1)	0.009(1)	-0.002(1)
C1	0.026(1)	0.047(2)	0.035(1)	-0.001(1)	0.010(1)	-0.009(1)
C2	0.023(1)	0.034(1)	0.027(1)	0.001(1)	0.010(1)	-0.003(1)
C3	0.029(1)	0.028(1)	0.026(1)	0.000(1)	0.009(1)	-0.002(1)
C4	0.037(1)	0.035(1)	0.039(1)	0.002(1)	0.011(1)	0.003(1)
C5	0.022(1)	0.030(1)	0.023(1)	-0.004(1)	0.007(1)	-0.002(1)
C6	0.028(1)	0.025(1)	0.033(1)	0.003(1)	0.005(1)	-0.005(1)
C7	0.022(1)	0.030(1)	0.024(1)	-0.001(1)	0.007(1)	0.000(1)
C8	0.024(1)	0.030(1)	0.023(1)	-0.003(1)	0.007(1)	0.000(1)
C9	0.027(1)	0.034(1)	0.035(1)	-0.004(1)	0.013(1)	-0.002(1)
C10	0.030(1)	0.048(2)	0.033(1)	-0.002(1)	0.010(1)	0.002(1)
C11	0.023(1)	0.030(1)	0.031(1)	0.003(1)	0.011(1)	0.000(1)
C12	0.022(1)	0.038(1)	0.030(1)	-0.001(1)	0.007(1)	-0.004(1)
C13	0.030(1)	0.049(2)	0.035(1)	0.002(1)	0.017(1)	0.005(1)
C14	0.031(1)	0.042(2)	0.028(1)	-0.002(1)	0.011(1)	-0.004(1)
C15	0.031(1)	0.033(1)	0.035(1)	-0.001(1)	0.012(1)	0.002(1)
C16	0.028(1)	0.035(1)	0.045(2)	0.000(1)	0.010(1)	-0.006(1)
C17	0.043(2)	0.054(2)	0.043(2)	0.019(1)	0.020(1)	0.004(1)
C18	0.037(2)	0.040(2)	0.040(2)	-0.002(1)	0.004(1)	0.000(1)
C19	0.054(2)	0.065(2)	0.037(2)	-0.023(2)	0.005(1)	0.013(2)
C20	0.029(1)	0.035(1)	0.032(1)	0.003(1)	0.011(1)	-0.002(1)
C21	0.063(2)	0.069(2)	0.047(2)	0.027(2)	0.036(2)	0.023(2)
C22	0.044(2)	0.057(2)	0.039(2)	0.005(1)	0.025(1)	0.003(1)
C23	0.034(2)	0.052(2)	0.041(2)	0.008(1)	-0.004(1)	-0.006(1)
C24	0.025(1)	0.026(1)	0.022(1)	-0.003(1)	0.007(1)	0.000(1)
C25	0.031(1)	0.035(2)	0.044(2)	0.008(1)	0.007(1)	-0.001(1)
C26	0.024(1)	0.032(1)	0.050(2)	-0.001(1)	0.003(1)	0.001(1)
C27	0.025(1)	0.036(2)	0.060(2)	0.006(1)	0.005(1)	-0.002(1)
C28	0.029(2)	0.039(2)	0.088(2)	0.019(2)	0.002(2)	-0.003(1)
C29	0.023(1)	0.028(1)	0.024(1)	-0.002(1)	0.006(1)	-0.005(1)
C30	0.040(2)	0.049(2)	0.043(2)	-0.025(1)	0.009(1)	0.004(1)
C31	0.026(1)	0.047(2)	0.047(2)	0.008(1)	0.016(1)	-0.003(1)
C32	0.045(2)	0.039(2)	0.096(3)	-0.033(2)	0.018(2)	-0.001(1)
C33	0.043(2)	0.073(2)	0.035(2)	0.000(2)	0.013(1)	0.021(2)
C34	0.042(2)	0.040(2)	0.036(1)	0.013(1)	0.009(1)	-0.002(1)
C35	0.036(2)	0.044(2)	0.079(2)	0.031(2)	0.014(2)	-0.001(1)
C36	0.045(2)	0.047(2)	0.030(1)	-0.006(1)	0.013(1)	-0.004(1)
C37	0.033(1)	0.057(2)	0.042(2)	0.008(1)	0.011(1)	0.011(1)

C38	0.043(2)	0.084(3)	0.093(3)	0.062(2)	0.040(2)	0.019(2)
C39	0.051(2)	0.049(2)	0.036(2)	-0.005(1)	0.003(1)	-0.014(2)
C40	0.039(2)	0.086(3)	0.077(2)	-0.062(2)	-0.006(2)	0.004(2)
C41	0.050(2)	0.043(2)	0.095(3)	-0.024(2)	0.011(2)	0.007(2)
C42	0.038(2)	0.045(2)	0.056(2)	-0.009(1)	0.006(1)	0.006(1)
C43	0.040(2)	0.053(2)	0.024(1)	0.006(1)	0.011(1)	-0.004(1)
C44	0.038(2)	0.064(2)	0.117(3)	0.051(2)	0.014(2)	-0.012(2)
C45	0.031(1)	0.061(2)	0.042(2)	0.005(1)	0.019(1)	-0.006(1)
C46	0.036(2)	0.032(2)	0.129(4)	-0.003(2)	0.005(2)	0.000(1)
C47	0.051(2)	0.045(2)	0.047(2)	-0.012(1)	0.009(1)	0.002(1)
C48	0.036(2)	0.077(2)	0.040(2)	0.016(2)	0.012(1)	0.012(2)
C49	0.043(2)	0.052(2)	0.124(3)	-0.053(2)	0.022(2)	-0.015(2)
C50	0.057(2)	0.100(3)	0.031(2)	0.010(2)	0.018(1)	0.030(2)

The general temperature factor expression:

$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Zr1	C8	2.235(2)	Zr1	C7	2.350(2)
Zr1	C35	2.492(3)	Zr1	C44	2.493(3)
Zr1	C38	2.512(3)	Zr1	C17	2.518(3)
Zr1	C21	2.534(3)	Zr1	C49	2.535(3)
Zr1	C40	2.541(3)	Zr1	C19	2.545(3)
Zr1	C32	2.549(3)	Zr1	C30	2.556(3)
P1	C6	1.838(3)	P1	C7	1.838(2)
P1	C26	1.843(3)	P2	C8	1.744(2)
P2	C2	1.820(2)	P2	C12	1.838(3)
C1	C45	1.390(4)	C1	C2	1.399(3)
C1	H1A	0.9300	C2	C20	1.377(3)
C3	C4	1.373(4)	C3	C29	1.389(3)
C3	H3A	0.9300	C4	C34	1.388(4)
C4	H4A	0.9300	C5	C7	1.368(3)
C5	C24	1.493(3)	C5	C11	1.503(3)
C6	C18	1.385(4)	C6	C25	1.400(3)
C8	C24	1.349(3)	C8	H8A	0.9800
C9	C16	1.389(3)	C9	C11	1.393(3)
C9	H9A	0.9300	C10	C37	1.371(4)
C10	C12	1.384(4)	C10	H10A	0.9300
C11	C15	1.404(3)	C12	C33	1.386(4)
C13	C31	1.381(4)	C13	C15	1.384(3)
C13	H13A	0.9300	C14	C43	1.382(4)
C14	C29	1.396(3)	C14	H14A	0.9300
C15	H15A	0.9300	C16	C31	1.382(4)
C16	H16A	0.9300	C17	C35	1.404(5)
C17	C21	1.410(4)	C17	H17A	0.9800
C18	C47	1.398(4)	C18	H18A	0.9300
C19	C40	1.411(5)	C19	C30	1.412(4)
C19	H19A	0.9800	C20	C36	1.397(3)
C20	H20A	0.9300	C21	C38	1.407(6)
C21	H21A	0.9800	C22	C45	1.377(4)
C22	C36	1.385(4)	C22	H22A	0.9300
C23	C25	1.371(4)	C23	C39	1.384(4)
C23	H23A	0.9300	C24	C29	1.493(3)
C25	H25A	0.9300	C26	C42	1.395(4)
C26	C27	1.397(4)	C27	C28	1.401(4)
C27	H27A	0.9300	C28	C46	1.370(5)
C28	H28A	0.9300	C30	C32	1.406(5)
C30	H30A	0.9800	C31	H31A	0.9300

C32	C49	1.425(5)	C32	H32A	0.9800
C33	C50	1.378(4)	C33	H33A	0.9300
C34	C43	1.377(4)	C34	H34A	0.9300
C35	C44	1.420(4)	C35	H35A	0.9800
C36	H36A	0.9300	C37	C48	1.379(4)
C37	H37A	0.9300	C38	C44	1.376(6)
C38	H38A	0.9800	C39	C47	1.369(4)
C39	H39A	0.9300	C40	C49	1.386(6)
C40	H40A	0.9800	C41	C46	1.374(6)
C41	C42	1.388(5)	C41	H41A	0.9300
C42	H42A	0.9300	C43	H43A	0.9300
C44	H44A	0.9800	C45	H45A	0.9300
C46	H46A	0.9300	C47	H47A	0.9300
C48	C50	1.382(4)	C48	H48A	0.9300
C49	H49A	0.9800	C50	H50A	0.9300

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C8	Zr1	C7	71.28(8)	C8	Zr1	C35	135.05(11)
C7	Zr1	C35	98.87(9)	C8	Zr1	C44	128.19(12)
C7	Zr1	C44	130.76(10)	C35	Zr1	C44	33.10(10)
C8	Zr1	C38	96.28(11)	C7	Zr1	C38	127.15(12)
C35	Zr1	C38	54.02(11)	C44	Zr1	C38	31.91(13)
C8	Zr1	C17	103.75(10)	C7	Zr1	C17	79.10(9)
C35	Zr1	C17	32.54(11)	C44	Zr1	C17	53.74(12)
C38	Zr1	C17	53.52(11)	C8	Zr1	C21	82.43(10)
C7	Zr1	C21	94.92(10)	C35	Zr1	C21	54.13(12)
C44	Zr1	C21	53.51(14)	C38	Zr1	C21	32.37(13)
C17	Zr1	C21	32.42(10)	C8	Zr1	C49	132.27(13)
C7	Zr1	C49	123.21(10)	C35	Zr1	C49	90.50(15)
C44	Zr1	C49	79.73(16)	C38	Zr1	C49	103.43(14)
C17	Zr1	C49	122.99(14)	C21	Zr1	C49	132.95(14)
C8	Zr1	C40	100.64(12)	C7	Zr1	C40	117.76(11)
C35	Zr1	C40	121.56(14)	C44	Zr1	C40	103.31(15)
C38	Zr1	C40	114.99(14)	C17	Zr1	C40	153.98(14)
C21	Zr1	C40	146.57(12)	C49	Zr1	C40	31.70(14)
C8	Zr1	C19	87.70(10)	C7	Zr1	C19	85.72(10)
C35	Zr1	C19	136.35(12)	C44	Zr1	C19	132.59(14)
C38	Zr1	C19	146.44(13)	C17	Zr1	C19	156.72(10)
C21	Zr1	C19	169.32(11)	C49	Zr1	C19	53.13(13)
C40	Zr1	C19	32.21(12)	C8	Zr1	C32	139.72(11)
C7	Zr1	C32	93.10(9)	C35	Zr1	C32	82.87(13)
C44	Zr1	C32	90.42(14)	C38	Zr1	C32	121.60(13)
C17	Zr1	C32	109.48(12)	C21	Zr1	C32	136.97(12)
C49	Zr1	C32	32.55(10)	C40	Zr1	C32	53.31(12)
C19	Zr1	C32	53.49(12)	C8	Zr1	C30	108.81(9)
C7	Zr1	C30	71.18(9)	C35	Zr1	C30	108.79(11)
C44	Zr1	C30	122.34(13)	C38	Zr1	C30	153.46(13)
C17	Zr1	C30	124.89(10)	C21	Zr1	C30	157.10(10)
C49	Zr1	C30	52.99(11)	C40	Zr1	C30	52.93(10)
C19	Zr1	C30	32.13(10)	C32	Zr1	C30	31.98(11)
C6	P1	C7	102.40(11)	C6	P1	C26	102.97(12)
C7	P1	C26	108.42(11)	C8	P2	C2	109.83(11)
C8	P2	C12	117.21(11)	C2	P2	C12	104.09(11)
C8	P2	Zr1	52.40(8)	C2	P2	Zr1	116.29(8)
C12	P2	Zr1	139.50(8)	C45	C1	C2	120.2(3)
C45	C1	H1A	119.9	C2	C1	H1A	119.9

C20	C2	C1	119.3(2)	C20	C2	P2	122.32(17)
C1	C2	P2	118.36(19)	C4	C3	C29	121.5(2)
C4	C3	H3A	119.2	C29	C3	H3A	119.2
C3	C4	C34	119.9(3)	C3	C4	H4A	120.0
C34	C4	H4A	120.0	C7	C5	C24	116.9(2)
C7	C5	C11	125.9(2)	C24	C5	C11	117.2(2)
C18	C6	C25	117.6(2)	C18	C6	P1	123.4(2)
C25	C6	P1	118.5(2)	C5	C7	P1	113.11(16)
C5	C7	Zr1	110.96(15)	P1	C7	Zr1	135.38(12)
C24	C8	P2	134.99(19)	C24	C8	Zr1	114.42(16)
P2	C8	Zr1	89.43(10)	C24	C8	H8A	104.8
P2	C8	H8A	104.8	Zr1	C8	H8A	104.8
C16	C9	C11	120.7(2)	C16	C9	H9A	119.6
C11	C9	H9A	119.6	C37	C10	C12	121.3(2)
C37	C10	H10A	119.4	C12	C10	H10A	119.4
C9	C11	C15	118.4(2)	C9	C11	C5	121.2(2)
C15	C11	C5	120.2(2)	C10	C12	C33	117.7(2)
C10	C12	P2	121.80(18)	C33	C12	P2	120.4(2)
C31	C13	C15	120.2(2)	C31	C13	H13A	119.9
C15	C13	H13A	119.9	C43	C14	C29	120.3(2)
C43	C14	H14A	119.8	C29	C14	H14A	119.8
C13	C15	C11	120.5(2)	C13	C15	H15A	119.7
C11	C15	H15A	119.7	C31	C16	C9	120.0(3)
C31	C16	H16A	120.0	C9	C16	H16A	120.0
C35	C17	C21	108.7(3)	C35	C17	Zr1	72.72(18)
C21	C17	Zr1	74.41(17)	C35	C17	H17A	125.4
C21	C17	H17A	125.4	Zr1	C17	H17A	125.4
C6	C18	C47	120.7(3)	C6	C18	H18A	119.6
C47	C18	H18A	119.6	C40	C19	C30	107.2(3)
C40	C19	Zr1	73.75(19)	C30	C19	Zr1	74.37(18)
C40	C19	H19A	126.0	C30	C19	H19A	126.0
Zr1	C19	H19A	126.0	C2	C20	C36	120.5(2)
C2	C20	H20A	119.7	C36	C20	H20A	119.7
C38	C21	C17	107.0(3)	C38	C21	Zr1	73.0(2)
C17	C21	Zr1	73.18(17)	C38	C21	H21A	126.2
C17	C21	H21A	126.2	Zr1	C21	H21A	126.2
C45	C22	C36	120.4(2)	C45	C22	H22A	119.8
C36	C22	H22A	119.8	C25	C23	C39	120.5(3)
C25	C23	H23A	119.7	C39	C23	H23A	119.7
C8	C24	C29	122.8(2)	C8	C24	C5	114.2(2)
C29	C24	C5	122.95(19)	C23	C25	C6	121.3(3)
C23	C25	H25A	119.3	C6	C25	H25A	119.3
C42	C26	C27	117.4(3)	C42	C26	P1	116.5(2)
C27	C26	P1	125.8(2)	C26	C27	C28	120.4(3)
C26	C27	H27A	119.8	C28	C27	H27A	119.8
C46	C28	C27	120.9(3)	C46	C28	H28A	119.6

C27	C28	H28A	119.6	C3	C29	C14	118.1(2)
C3	C29	C24	118.84(19)	C14	C29	C24	123.0(2)
C32	C30	C19	108.9(3)	C32	C30	Zr1	73.73(17)
C19	C30	Zr1	73.50(17)	C32	C30	H30A	125.3
C19	C30	H30A	125.3	Zr1	C30	H30A	125.3
C13	C31	C16	120.2(2)	C13	C31	H31A	119.9
C16	C31	H31A	119.9	C30	C32	C49	106.7(3)
C30	C32	Zr1	74.29(16)	C49	C32	Zr1	73.21(17)
C30	C32	H32A	126.2	C49	C32	H32A	126.2
Zr1	C32	H32A	126.2	C50	C33	C12	121.2(3)
C50	C33	H33A	119.4	C12	C33	H33A	119.4
C43	C34	C4	119.3(3)	C43	C34	H34A	120.4
C4	C34	H34A	120.4	C17	C35	C44	106.6(3)
C17	C35	Zr1	74.73(17)	C44	C35	Zr1	73.49(18)
C17	C35	H35A	126.2	C44	C35	H35A	126.2
Zr1	C35	H35A	126.2	C22	C36	C20	119.6(3)
C22	C36	H36A	120.2	C20	C36	H36A	120.2
C10	C37	C48	120.9(3)	C10	C37	H37A	119.6
C48	C37	H37A	119.6	C44	C38	C21	108.9(3)
C44	C38	Zr1	73.3(2)	C21	C38	Zr1	74.68(16)
C44	C38	H38A	125.3	C21	C38	H38A	125.3
Zr1	C38	H38A	125.3	C47	C39	C23	119.3(3)
C47	C39	H39A	120.4	C23	C39	H39A	120.4
C49	C40	C19	108.6(3)	C49	C40	Zr1	73.9(2)
C19	C40	Zr1	74.05(17)	C49	C40	H40A	125.4
C19	C40	H40A	125.4	Zr1	C40	H40A	125.4
C46	C41	C42	120.3(4)	C46	C41	H41A	119.9
C42	C41	H41A	119.9	C41	C42	C26	121.5(3)
C41	C42	H42A	119.3	C26	C42	H42A	119.3
C34	C43	C14	120.8(2)	C34	C43	H43A	119.6
C14	C43	H43A	119.6	C38	C44	C35	108.7(4)
C38	C44	Zr1	74.79(18)	C35	C44	Zr1	73.41(17)
C38	C44	H44A	125.3	C35	C44	H44A	125.3
Zr1	C44	H44A	125.3	C22	C45	C1	119.9(2)
C22	C45	H45A	120.0	C1	C45	H45A	120.0
C28	C46	C41	119.5(3)	C28	C46	H46A	120.3
C41	C46	H46A	120.3	C39	C47	C18	120.5(3)
C39	C47	H47A	119.7	C18	C47	H47A	119.7
C37	C48	C50	118.5(3)	C37	C48	H48A	120.8
C50	C48	H48A	120.8	C40	C49	C32	108.6(3)
C40	C49	Zr1	74.37(18)	C32	C49	Zr1	74.23(17)
C40	C49	H49A	125.3	C32	C49	H49A	125.3
Zr1	C49	H49A	125.3	C33	C50	C48	120.5(3)
C33	C50	H50A	119.7	C48	C50	H50A	119.7

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C7	Zr1	P2	C8	8.20(11)	C35	Zr1	P2	C8	-113.60(14)
C44	Zr1	P2	C8	-135.06(14)	C38	Zr1	P2	C8	-117.17(14)
C17	Zr1	P2	C8	-78.76(12)	C21	Zr1	P2	C8	-85.04(13)
C49	Zr1	P2	C8	141.98(14)	C40	Zr1	P2	C8	123.90(14)
C19	Zr1	P2	C8	92.07(13)	C32	Zr1	P2	C8	121.06(14)
C30	Zr1	P2	C8	86.29(12)	C8	Zr1	P2	C2	95.57(13)
C7	Zr1	P2	C2	103.77(11)	C35	Zr1	P2	C2	-18.03(14)
C44	Zr1	P2	C2	-39.49(14)	C38	Zr1	P2	C2	-21.60(14)
C17	Zr1	P2	C2	16.81(12)	C21	Zr1	P2	C2	10.53(13)
C49	Zr1	P2	C2	-122.45(14)	C40	Zr1	P2	C2	-140.53(14)
C19	Zr1	P2	C2	-172.36(12)	C32	Zr1	P2	C2	-143.37(14)
C30	Zr1	P2	C2	-178.14(12)	C8	Zr1	P2	C12	-89.25(16)
C7	Zr1	P2	C12	-81.05(14)	C35	Zr1	P2	C12	157.15(16)
C44	Zr1	P2	C12	135.69(16)	C38	Zr1	P2	C12	153.58(17)
C17	Zr1	P2	C12	-168.00(15)	C21	Zr1	P2	C12	-174.28(15)
C49	Zr1	P2	C12	52.73(16)	C40	Zr1	P2	C12	34.65(16)
C19	Zr1	P2	C12	2.82(15)	C32	Zr1	P2	C12	31.82(17)
C30	Zr1	P2	C12	-2.96(15)	C45	C1	C2	C20	0.2(4)
C45	C1	C2	P2	-178.4(2)	C8	P2	C2	C20	-16.5(3)
C12	P2	C2	C20	109.8(2)	Zr1	P2	C2	C20	-73.5(2)
C8	P2	C2	C1	162.1(2)	C12	P2	C2	C1	-71.7(2)
Zr1	P2	C2	C1	105.1(2)	C29	C3	C4	C34	-0.6(4)
C7	P1	C6	C18	12.5(2)	C26	P1	C6	C18	125.0(2)
C7	P1	C6	C25	-175.68(19)	C26	P1	C6	C25	-63.2(2)
C24	C5	C7	P1	170.44(16)	C11	C5	C7	P1	-9.2(3)
C24	C5	C7	Zr1	-16.8(2)	C11	C5	C7	Zr1	163.65(18)
C6	P1	C7	C5	-88.06(18)	C26	P1	C7	C5	163.55(17)
C6	P1	C7	Zr1	101.52(16)	C26	P1	C7	Zr1	-6.9(2)
C8	Zr1	C7	C5	24.67(15)	C35	Zr1	C7	C5	159.37(17)
C44	Zr1	C7	C5	149.41(19)	C38	Zr1	C7	C5	108.26(18)
C17	Zr1	C7	C5	133.38(18)	C21	Zr1	C7	C5	104.96(17)
C49	Zr1	C7	C5	-104.2(2)	C40	Zr1	C7	C5	-67.7(2)
C19	Zr1	C7	C5	-64.35(17)	C32	Zr1	C7	C5	-117.36(18)
C30	Zr1	C7	C5	-93.70(17)	C8	Zr1	C7	P1	-164.76(18)
C35	Zr1	C7	P1	-30.06(18)	C44	Zr1	C7	P1	-40.0(2)
C38	Zr1	C7	P1	-81.18(19)	C17	Zr1	C7	P1	-56.05(16)
C21	Zr1	C7	P1	-84.48(17)	C49	Zr1	C7	P1	66.4(2)
C40	Zr1	C7	P1	102.83(18)	C19	Zr1	C7	P1	106.22(17)
C32	Zr1	C7	P1	53.20(18)	C30	Zr1	C7	P1	76.87(17)

C2	P2	C8	C24	126.5(3)	C12	P2	C8	C24	8.0(3)
Zr1	P2	C8	C24	-125.1(3)	C2	P2	C8	Zr1	-108.45(11)
C12	P2	C8	Zr1	133.10(10)	C7	Zr1	C8	C24	-31.29(17)
C35	Zr1	C8	C24	-115.03(18)	C44	Zr1	C8	C24	-158.92(18)
C38	Zr1	C8	C24	-158.46(19)	C17	Zr1	C8	C24	-104.53(18)
C21	Zr1	C8	C24	-129.13(19)	C49	Zr1	C8	C24	87.0(2)
C40	Zr1	C8	C24	84.60(19)	C19	Zr1	C8	C24	54.96(18)
C32	Zr1	C8	C24	40.5(2)	C30	Zr1	C8	C24	30.33(19)
C7	Zr1	C8	P2	-171.82(11)	C35	Zr1	C8	P2	104.44(13)
C44	Zr1	C8	P2	60.55(15)	C38	Zr1	C8	P2	61.02(12)
C17	Zr1	C8	P2	114.94(10)	C21	Zr1	C8	P2	90.34(11)
C49	Zr1	C8	P2	-53.56(16)	C40	Zr1	C8	P2	-55.92(12)
C19	Zr1	C8	P2	-85.56(11)	C32	Zr1	C8	P2	-99.98(14)
C30	Zr1	C8	P2	-110.20(10)	C16	C9	C11	C15	-0.6(4)
C16	C9	C11	C5	174.1(2)	C7	C5	C11	C9	121.3(3)
C24	C5	C11	C9	-58.3(3)	C7	C5	C11	C15	-64.1(3)
C24	C5	C11	C15	116.3(2)	C37	C10	C12	C33	-0.1(4)
C37	C10	C12	P2	-175.6(2)	C8	P2	C12	C10	110.0(2)
C2	P2	C12	C10	-11.5(2)	Zr1	P2	C12	C10	172.98(15)
C8	P2	C12	C33	-65.4(3)	C2	P2	C12	C33	173.1(2)
Zr1	P2	C12	C33	-2.4(3)	C31	C13	C15	C11	0.4(4)
C9	C11	C15	C13	0.6(4)	C5	C11	C15	C13	-174.2(2)
C11	C9	C16	C31	-0.3(4)	C8	Zr1	C17	C35	-166.15(17)
C7	Zr1	C17	C35	126.40(19)	C44	Zr1	C17	C35	-38.57(19)
C38	Zr1	C17	C35	-78.5(2)	C21	Zr1	C17	C35	-115.8(3)
C49	Zr1	C17	C35	3.7(2)	C40	Zr1	C17	C35	-7.0(3)
C19	Zr1	C17	C35	76.2(3)	C32	Zr1	C17	C35	37.0(2)
C30	Zr1	C17	C35	68.7(2)	C8	Zr1	C17	C21	-50.3(2)
C7	Zr1	C17	C21	-117.8(2)	C35	Zr1	C17	C21	115.8(3)
C44	Zr1	C17	C21	77.3(2)	C38	Zr1	C17	C21	37.3(2)
C49	Zr1	C17	C21	119.5(2)	C40	Zr1	C17	C21	108.8(3)
C19	Zr1	C17	C21	-168.0(3)	C32	Zr1	C17	C21	152.8(2)
C30	Zr1	C17	C21	-175.4(2)	C25	C6	C18	C47	1.1(4)
P1	C6	C18	C47	173.0(2)	C8	Zr1	C19	C40	114.2(2)
C7	Zr1	C19	C40	-174.4(2)	C35	Zr1	C19	C40	-76.0(3)
C44	Zr1	C19	C40	-29.2(3)	C38	Zr1	C19	C40	16.3(3)
C17	Zr1	C19	C40	-125.2(3)	C21	Zr1	C19	C40	91.8(7)
C49	Zr1	C19	C40	-36.4(2)	C32	Zr1	C19	C40	-77.3(2)
C30	Zr1	C19	C40	-113.7(3)	C8	Zr1	C19	C30	-132.1(2)
C7	Zr1	C19	C30	-60.7(2)	C35	Zr1	C19	C30	37.7(3)
C44	Zr1	C19	C30	84.4(2)	C38	Zr1	C19	C30	130.0(2)
C17	Zr1	C19	C30	-11.5(4)	C21	Zr1	C19	C30	-154.6(6)
C49	Zr1	C19	C30	77.3(2)	C40	Zr1	C19	C30	113.7(3)
C32	Zr1	C19	C30	36.34(18)	C1	C2	C20	C36	-1.4(4)
P2	C2	C20	C36	177.1(2)	C35	C17	C21	C38	-0.4(3)
Zr1	C17	C21	C38	-65.6(2)	C35	C17	C21	Zr1	65.2(2)

C8	Zr1	C21	C38	-114.6(2)	C7	Zr1	C21	C38	175.1(2)
C35	Zr1	C21	C38	77.7(2)	C44	Zr1	C21	C38	36.36(19)
C17	Zr1	C21	C38	114.4(3)	C49	Zr1	C21	C38	28.9(3)
C40	Zr1	C21	C38	-16.7(3)	C19	Zr1	C21	C38	-91.9(7)
C32	Zr1	C21	C38	75.2(2)	C30	Zr1	C21	C38	124.0(3)
C8	Zr1	C21	C17	131.0(2)	C7	Zr1	C21	C17	60.7(2)
C35	Zr1	C21	C17	-36.70(18)	C44	Zr1	C21	C17	-78.0(2)
C38	Zr1	C21	C17	-114.4(3)	C49	Zr1	C21	C17	-85.5(2)
C40	Zr1	C21	C17	-131.1(3)	C19	Zr1	C21	C17	153.7(6)
C32	Zr1	C21	C17	-39.2(3)	C30	Zr1	C21	C17	9.6(4)
P2	C8	C24	C29	-28.2(4)	Zr1	C8	C24	C29	-144.21(18)
P2	C8	C24	C5	149.3(2)	Zr1	C8	C24	C5	33.3(2)
C7	C5	C24	C8	-9.7(3)	C11	C5	C24	C8	169.9(2)
C7	C5	C24	C29	167.8(2)	C11	C5	C24	C29	-12.6(3)
C39	C23	C25	C6	0.5(4)	C18	C6	C25	C23	-0.9(4)
P1	C6	C25	C23	-173.2(2)	C6	P1	C26	C42	158.6(2)
C7	P1	C26	C42	-93.4(2)	C6	P1	C26	C27	-14.8(2)
C7	P1	C26	C27	93.2(2)	C42	C26	C27	C28	2.1(4)
P1	C26	C27	C28	175.4(2)	C26	C27	C28	C46	0.3(4)
C4	C3	C29	C14	0.8(4)	C4	C3	C29	C24	178.0(2)
C43	C14	C29	C3	-0.1(4)	C43	C14	C29	C24	-177.2(2)
C8	C24	C29	C3	-42.5(3)	C5	C24	C29	C3	140.2(2)
C8	C24	C29	C14	134.5(2)	C5	C24	C29	C14	-42.8(3)
C40	C19	C30	C32	1.2(3)	Zr1	C19	C30	C32	-65.8(2)
C40	C19	C30	Zr1	67.0(2)	C8	Zr1	C30	C32	167.49(18)
C7	Zr1	C30	C32	-130.8(2)	C35	Zr1	C30	C32	-37.6(2)
C44	Zr1	C30	C32	-3.9(2)	C38	Zr1	C30	C32	7.4(3)
C17	Zr1	C30	C32	-69.6(2)	C21	Zr1	C30	C32	-75.9(3)
C49	Zr1	C30	C32	38.2(2)	C40	Zr1	C30	C32	78.2(2)
C19	Zr1	C30	C32	115.9(3)	C8	Zr1	C30	C19	51.5(2)
C7	Zr1	C30	C19	113.2(2)	C35	Zr1	C30	C19	-153.6(2)
C44	Zr1	C30	C19	-119.9(2)	C38	Zr1	C30	C19	-108.6(3)
C17	Zr1	C30	C19	174.5(2)	C21	Zr1	C30	C19	168.2(3)
C49	Zr1	C30	C19	-77.7(2)	C40	Zr1	C30	C19	-37.7(2)
C32	Zr1	C30	C19	-115.9(3)	C15	C13	C31	C16	-1.3(4)
C9	C16	C31	C13	1.3(4)	C19	C30	C32	C49	-0.9(3)
Zr1	C30	C32	C49	-66.6(2)	C19	C30	C32	Zr1	65.6(2)
C8	Zr1	C32	C30	-18.5(3)	C7	Zr1	C32	C30	45.84(19)
C35	Zr1	C32	C30	144.40(19)	C44	Zr1	C32	C30	176.70(19)
C38	Zr1	C32	C30	-176.15(17)	C17	Zr1	C32	C30	125.37(19)
C21	Zr1	C32	C30	146.43(19)	C49	Zr1	C32	C30	-113.3(3)
C40	Zr1	C32	C30	-76.9(2)	C19	Zr1	C32	C30	-36.52(18)
C8	Zr1	C32	C49	94.9(3)	C7	Zr1	C32	C49	159.2(3)
C35	Zr1	C32	C49	-102.3(3)	C44	Zr1	C32	C49	-69.9(3)
C38	Zr1	C32	C49	-62.8(3)	C17	Zr1	C32	C49	-121.3(3)
C21	Zr1	C32	C49	-100.2(3)	C40	Zr1	C32	C49	36.4(3)

C19	Zr1	C32	C49	76.8(3)	C30	Zr1	C32	C49	113.3(3)
C10	C12	C33	C50	0.2(5)	P2	C12	C33	C50	175.8(3)
C3	C4	C34	C43	-0.2(4)	C21	C17	C35	C44	0.8(3)
Zr1	C17	C35	C44	67.1(2)	C21	C17	C35	Zr1	-66.3(2)
C8	Zr1	C35	C17	19.2(2)	C7	Zr1	C35	C17	-53.12(19)
C44	Zr1	C35	C17	113.0(3)	C38	Zr1	C35	C17	76.8(2)
C21	Zr1	C35	C17	36.55(18)	C49	Zr1	C35	C17	-176.88(19)
C40	Zr1	C35	C17	176.41(17)	C19	Zr1	C35	C17	-146.22(19)
C32	Zr1	C35	C17	-145.16(19)	C30	Zr1	C35	C17	-126.15(18)
C8	Zr1	C35	C44	-93.8(3)	C7	Zr1	C35	C44	-166.1(2)
C38	Zr1	C35	C44	-36.2(3)	C17	Zr1	C35	C44	-113.0(3)
C21	Zr1	C35	C44	-76.4(3)	C49	Zr1	C35	C44	70.1(3)
C40	Zr1	C35	C44	63.4(3)	C19	Zr1	C35	C44	100.8(3)
C32	Zr1	C35	C44	101.9(3)	C30	Zr1	C35	C44	120.9(2)
C45	C22	C36	C20	0.2(4)	C2	C20	C36	C22	1.2(4)
C12	C10	C37	C48	-0.1(5)	C17	C21	C38	C44	-0.1(4)
Zr1	C21	C38	C44	-65.9(3)	C17	C21	C38	Zr1	65.76(19)
C8	Zr1	C38	C44	-179.3(2)	C7	Zr1	C38	C44	109.5(3)
C35	Zr1	C38	C44	37.6(2)	C17	Zr1	C38	C44	78.2(2)
C21	Zr1	C38	C44	115.6(3)	C49	Zr1	C38	C44	-43.1(3)
C40	Zr1	C38	C44	-74.5(3)	C19	Zr1	C38	C44	-84.0(3)
C32	Zr1	C38	C44	-13.6(3)	C30	Zr1	C38	C44	-18.2(4)
C8	Zr1	C38	C21	65.1(2)	C7	Zr1	C38	C21	-6.2(2)
C35	Zr1	C38	C21	-78.0(2)	C44	Zr1	C38	C21	-115.6(3)
C17	Zr1	C38	C21	-37.39(19)	C49	Zr1	C38	C21	-158.7(2)
C40	Zr1	C38	C21	169.9(2)	C19	Zr1	C38	C21	160.4(2)
C32	Zr1	C38	C21	-129.2(2)	C30	Zr1	C38	C21	-133.8(3)
C25	C23	C39	C47	-0.2(5)	C30	C19	C40	C49	-1.0(3)
Zr1	C19	C40	C49	66.4(2)	C30	C19	C40	Zr1	-67.4(2)
C8	Zr1	C40	C49	176.7(2)	C7	Zr1	C40	C49	-109.0(2)
C35	Zr1	C40	C49	12.8(3)	C44	Zr1	C40	C49	43.0(2)
C38	Zr1	C40	C49	74.5(2)	C17	Zr1	C40	C49	17.2(4)
C21	Zr1	C40	C49	84.3(3)	C19	Zr1	C40	C49	-115.3(3)
C32	Zr1	C40	C49	-37.4(2)	C30	Zr1	C40	C49	-77.7(2)
C8	Zr1	C40	C19	-68.0(2)	C7	Zr1	C40	C19	6.3(3)
C35	Zr1	C40	C19	128.2(2)	C44	Zr1	C40	C19	158.3(2)
C38	Zr1	C40	C19	-170.1(2)	C17	Zr1	C40	C19	132.6(3)
C21	Zr1	C40	C19	-160.4(2)	C49	Zr1	C40	C19	115.3(3)
C32	Zr1	C40	C19	77.9(2)	C30	Zr1	C40	C19	37.63(19)
C46	C41	C42	C26	1.2(5)	C27	C26	C42	C41	-2.8(4)
P1	C26	C42	C41	-176.8(2)	C4	C34	C43	C14	0.9(4)
C29	C14	C43	C34	-0.7(4)	C21	C38	C44	C35	0.7(4)
Zr1	C38	C44	C35	-66.1(2)	C21	C38	C44	Zr1	66.8(2)
C17	C35	C44	C38	-0.9(4)	Zr1	C35	C44	C38	67.0(3)
C17	C35	C44	Zr1	-68.0(2)	C8	Zr1	C44	C38	0.9(3)
C7	Zr1	C44	C38	-97.1(2)	C35	Zr1	C44	C38	-115.4(4)

C17	Zr1	C44	C38	-77.5(3)	C21	Zr1	C44	C38	-36.9(2)
C49	Zr1	C44	C38	137.5(3)	C40	Zr1	C44	C38	116.2(2)
C19	Zr1	C44	C38	131.7(2)	C32	Zr1	C44	C38	168.4(2)
C30	Zr1	C44	C38	170.5(2)	C8	Zr1	C44	C35	116.2(2)
C7	Zr1	C44	C35	18.2(3)	C38	Zr1	C44	C35	115.4(4)
C17	Zr1	C44	C35	37.9(2)	C21	Zr1	C44	C35	78.5(2)
C49	Zr1	C44	C35	-107.1(3)	C40	Zr1	C44	C35	-128.5(2)
C19	Zr1	C44	C35	-112.9(2)	C32	Zr1	C44	C35	-76.2(2)
C30	Zr1	C44	C35	-74.1(3)	C36	C22	C45	C1	-1.5(5)
C2	C1	C45	C22	1.3(4)	C27	C28	C46	C41	-2.0(5)
C42	C41	C46	C28	1.3(5)	C23	C39	C47	C18	0.4(5)
C6	C18	C47	C39	-0.9(5)	C10	C37	C48	C50	0.2(5)
C19	C40	C49	C32	0.4(4)	Zr1	C40	C49	C32	66.9(2)
C19	C40	C49	Zr1	-66.5(2)	C30	C32	C49	C40	0.3(4)
Zr1	C32	C49	C40	-67.0(2)	C30	C32	C49	Zr1	67.3(2)
C8	Zr1	C49	C40	-4.4(3)	C7	Zr1	C49	C40	90.0(2)
C35	Zr1	C49	C40	-169.1(2)	C44	Zr1	C49	C40	-137.6(2)
C38	Zr1	C49	C40	-116.1(2)	C17	Zr1	C49	C40	-171.1(2)
C21	Zr1	C49	C40	-131.5(2)	C19	Zr1	C49	C40	37.0(2)
C32	Zr1	C49	C40	115.1(4)	C30	Zr1	C49	C40	77.5(2)
C8	Zr1	C49	C32	-119.5(2)	C7	Zr1	C49	C32	-25.1(3)
C35	Zr1	C49	C32	75.9(3)	C44	Zr1	C49	C32	107.3(3)
C38	Zr1	C49	C32	128.8(2)	C17	Zr1	C49	C32	73.9(3)
C21	Zr1	C49	C32	113.4(2)	C40	Zr1	C49	C32	-115.1(4)
C19	Zr1	C49	C32	-78.0(3)	C30	Zr1	C49	C32	-37.5(2)
C12	C33	C50	C48	-0.1(6)	C37	C48	C50	C33	-0.1(5)

X-Ray Structural Data for 8:

Data Collection

A fragment of a red block-like crystal of C30 H39 P Zr having approximate dimensions of 0.23 x 0.16 x 0.09 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker Apex [10] CCD area detector with graphite monochromated MoKradiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 3127 centered reflections with $I > 10\sigma(I)$ in the range $3.61 < \theta < 24.23^{o}$ corresponded to a primitive Monoclinic cell with dimensions:

a = 13.728(2) Å	$\alpha = 90^{o}$
b = 9.857(1) Å	$\beta = 109.002(2)^{o}$
c = 20.224(3) Å	$\gamma = 90^{o}$
V = 8876(1) Å^3	

For Z = 4 and F.W. = 521.80, the calculated density is 1.339 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

P2(1)/c

The data were collected at a temperature of 159(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3^{o} counted for a total of 30 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[11] to a maximum θ value of 24.71^{o}. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 0.97, Tmin = 0.91). Of the 11281 reflections that were collected, 4361 were unique (R_{int} = 0.0290); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the

rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 4361 reflections (all data) and 289 variable parameters and converged (largest parameter shift was 0.001 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0365 \text{ for 3322 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.0851$$

The standard deviation of an observation of unit weight[4] was 1.026. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.702 and -0.271 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[9] crystallographic software package of Bruker Analytical X-ray Systems Inc.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C30 H39 P Zr
Formula Weight	521.80
Crystal Color, Habit	red, block
Crystal Dimensions	0.23 x 0.16 x 0.09 mm
Crystal System	Monoclinic
Lattice Type	primitive
Lattice Parameters	a = 13.728(2) Å b = 9.857(1) Å c = 20.224(3) Å α= 90 ^{o} β= 109.002(2) ^{o} γ = 90^o V = 2587.5(6) $Å^3$
Space Group	P2(1)/c
Z value	4
D_{calc}	1.339 g/cm^3

F_{000}	1096
μ(MoK)	0.50 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker Apex
Radiation	MoK(λ = 0.71073 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	30 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
θ_{max}	24.71°
No. of Reflections Measured	Total: 11281 Unique: 4361 (R_{int} = 0.0290)
Corrections	Lorentz-polarization Absorption (Tmax = 0.97, Tmin = 0.91)

C. Structure Solution and Refinement

Structure Solution	direct (SHELXS-97 (Sheldrick, 1990))
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|F_o\|^2 - \|F_c\|^2)^2$
Least Squares Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (qP)^2 + 0.000P]$ where $P = [F_o^2 + 2F_c^2]/3$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	3322
No. Variables	289
Residuals: R; wR_2; Rall	0.0365; 0.0851; 0.0566
Goodness of Fit Indicator	1.026
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.702 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.271 $e^-/Å^3$

Table 1. Atomic coordinates and U_{iso}/U_{eq} and occupancy

atom	x	y	z	U_{eq}	Occupancy
Zr1	-0.2339(1)	0.1846(1)	-0.1656(1)	0.024(1)	1
C1	-0.2469(2)	0.4209(3)	-0.1498(2)	0.025(1)	1
C28	-0.3264(3)	0.1149(4)	-0.3864(2)	0.042(1)	1
P1	-0.2264(1)	0.1406(1)	-0.2995(1)	0.026(1)	1
C5	-0.4287(2)	0.1885(3)	-0.2187(2)	0.038(1)	1
C19	-0.2821(2)	0.5006(3)	-0.3395(2)	0.024(1)	1
C2	-0.2652(2)	0.4987(3)	-0.2072(2)	0.024(1)	1
C14	-0.0402(2)	0.1842(3)	-0.1310(2)	0.034(1)	1
C27	-0.0977(3)	0.1895(3)	-0.3823(2)	0.042(1)	1
C24	-0.2041(2)	0.5278(3)	-0.3677(2)	0.029(1)	1
C4	-0.2281(2)	0.2976(3)	-0.2608(2)	0.025(1)	1
C3	-0.2574(2)	0.4289(3)	-0.2706(2)	0.025(1)	1
C18	-0.2048(3)	0.7406(3)	-0.2195(2)	0.041(1)	1
C22	-0.3247(3)	0.6331(3)	-0.4678(2)	0.036(1)	1
C9	-0.3999(3)	0.0505(3)	-0.2159(2)	0.039(1)	1
C13	-0.0691(2)	0.0483(3)	-0.1320(2)	0.032(1)	1
C7	-0.3626(3)	0.1262(4)	-0.1047(2)	0.040(1)	1
C25	-0.1003(3)	0.1216(3)	-0.3153(2)	0.032(1)	1
C29	-0.4310(3)	0.1725(4)	-0.3918(2)	0.058(1)	1
C26	-0.0626(3)	-0.0252(3)	-0.3122(2)	0.045(1)	1
C23	-0.2256(3)	0.5942(3)	-0.4311(2)	0.037(1)	1
C21	-0.4032(3)	0.6066(3)	-0.4406(2)	0.036(1)	1
C20	-0.3817(2)	0.5420(3)	-0.3767(2)	0.029(1)	1
C15	-0.2528(3)	0.4827(3)	-0.0814(2)	0.034(1)	1
C17	-0.2915(3)	0.6498(3)	-0.2126(2)	0.031(1)	1
C12	-0.1119(3)	0.0269(4)	-0.0799(2)	0.042(1)	1
C8	-0.3589(3)	0.0127(4)	-0.1461(2)	0.040(1)	1
C16	-0.1648(3)	0.5800(4)	-0.0446(2)	0.043(1)	1
C11	-0.1090(3)	0.1493(5)	-0.0451(2)	0.052(1)	1
C10	-0.0638(3)	0.2461(4)	-0.0764(2)	0.048(1)	1
C6	-0.4070(3)	0.2336(4)	-0.1498(2)	0.039(1)	1
C30	-0.3362(3)	-0.0344(4)	-0.4062(2)	0.075(2)	1

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr1	0.022(1)	0.020(1)	0.028(1)	0.000(1)	0.006(1)	-0.001(1)
C1	0.017(2)	0.024(2)	0.029(2)	-0.008(1)	0.000(1)	-0.002(1)
C28	0.037(2)	0.048(2)	0.036(2)	-0.004(2)	0.005(2)	-0.002(2)
P1	0.028(1)	0.023(1)	0.027(1)	-0.003(1)	0.007(1)	0.000(1)
C5	0.018(2)	0.043(2)	0.050(2)	0.001(2)	0.007(2)	-0.005(2)
C19	0.029(2)	0.014(1)	0.031(2)	-0.004(1)	0.010(2)	-0.001(1)
C2	0.020(2)	0.020(2)	0.031(2)	-0.004(1)	0.007(1)	-0.003(1)
C14	0.022(2)	0.032(2)	0.043(2)	0.004(2)	0.003(2)	-0.003(2)
C27	0.045(2)	0.040(2)	0.047(2)	0.001(2)	0.024(2)	0.002(2)
C24	0.024(2)	0.030(2)	0.033(2)	0.000(1)	0.008(2)	0.002(1)
C4	0.023(2)	0.025(2)	0.025(2)	-0.002(1)	0.006(1)	0.001(1)
C3	0.018(2)	0.025(2)	0.031(2)	0.001(1)	0.007(1)	0.000(1)
C18	0.045(2)	0.022(2)	0.053(2)	-0.001(2)	0.013(2)	-0.002(2)
C22	0.048(2)	0.032(2)	0.026(2)	0.003(1)	0.009(2)	0.001(2)
C9	0.030(2)	0.038(2)	0.052(2)	-0.014(2)	0.015(2)	-0.017(2)
C13	0.021(2)	0.028(2)	0.042(2)	-0.003(2)	0.004(2)	0.005(1)
C7	0.034(2)	0.047(2)	0.047(2)	-0.004(2)	0.022(2)	-0.011(2)
C25	0.031(2)	0.031(2)	0.037(2)	-0.005(2)	0.014(2)	0.003(2)
C29	0.051(3)	0.048(2)	0.056(3)	-0.008(2)	-0.008(2)	0.003(2)
C26	0.047(2)	0.040(2)	0.051(2)	0.003(2)	0.021(2)	0.015(2)
C23	0.039(2)	0.036(2)	0.038(2)	-0.002(2)	0.017(2)	-0.001(2)
C21	0.034(2)	0.031(2)	0.034(2)	0.002(2)	0.001(2)	0.005(2)
C20	0.026(2)	0.026(2)	0.035(2)	0.000(1)	0.009(2)	-0.001(1)
C15	0.038(2)	0.029(2)	0.034(2)	-0.003(2)	0.012(2)	-0.001(2)
C17	0.033(2)	0.024(2)	0.036(2)	-0.001(1)	0.009(2)	0.005(1)
C12	0.035(2)	0.041(2)	0.046(2)	0.018(2)	0.008(2)	0.011(2)
C8	0.035(2)	0.031(2)	0.058(2)	-0.001(2)	0.021(2)	-0.012(2)
C16	0.049(2)	0.037(2)	0.040(2)	-0.009(2)	0.011(2)	-0.001(2)
C11	0.044(2)	0.081(3)	0.025(2)	0.002(2)	0.002(2)	0.018(2)
C10	0.032(2)	0.034(2)	0.055(2)	-0.018(2)	-0.018(2)	0.008(2)
C6	0.022(2)	0.034(2)	0.067(3)	-0.008(2)	0.023(2)	-0.006(2)
C30	0.058(3)	0.060(3)	0.081(3)	-0.040(2)	-0.011(3)	0.004(2)

The general temperature factor expression:

$$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Zr1	C4	2.248(3)	Zr1	C1	2.366(3)
Zr1	C11	2.506(3)	Zr1	C10	2.516(3)
Zr1	C12	2.517(3)	Zr1	C14	2.521(3)
Zr1	C13	2.527(3)	Zr1	C7	2.527(3)
Zr1	C8	2.532(3)	Zr1	C5	2.537(3)
Zr1	C9	2.543(3)	Zr1	C6	2.544(3)
C1	C2	1.344(4)	C1	C15	1.538(4)
C28	C29	1.515(5)	C28	C30	1.519(5)
C28	P1	1.862(3)	C28	H28A	0.9800
P1	C4	1.738(3)	P1	C25	1.870(3)
C5	C6	1.397(5)	C5	C9	1.413(5)
C5	H5A	0.9800	C19	C20	1.390(4)
C19	C24	1.393(4)	C19	C3	1.500(4)
C2	C3	1.489(4)	C2	C17	1.528(4)
C14	C10	1.391(5)	C14	C13	1.396(4)
C14	H14A	0.9800	C27	C25	1.521(5)
C27	H27A	0.9600	C27	H27B	0.9600
C27	H27C	0.9600	C24	C23	1.384(4)
C24	H24A	0.9300	C4	C3	1.351(4)
C18	C17	1.530(5)	C18	H18A	0.9600
C18	H18B	0.9600	C18	H18C	0.9600
C22	C23	1.375(5)	C22	C21	1.385(5)
C22	H22A	0.9300	C9	C8	1.390(5)
C9	H9A	0.9800	C13	C12	1.381(5)
C13	H13A	0.9800	C7	C6	1.401(5)
C7	C8	1.408(5)	C7	H7A	0.9800
C25	C26	1.530(4)	C25	H25A	0.9800
C29	H29A	0.9600	C29	H29B	0.9600
C29	H29C	0.9600	C26	H26A	0.9600
C26	H26B	0.9600	C26	H26C	0.9600
C23	H23A	0.9300	C21	C20	1.383(4)
C21	H21A	0.9300	C20	H20A	0.9300
C15	C16	1.532(4)	C15	H15A	0.9700
C15	H15B	0.9700	C17	H17A	0.9700
C17	H17B	0.9700	C12	C11	1.391(5)
C12	H12A	0.9800	C8	H8A	0.9800
C16	H16A	0.9600	C16	H16B	0.9600
C16	H16C	0.9600	C11	C10	1.396(6)
C11	H11A	0.9800	C10	H10A	0.9800
C6	H6A	0.9800	C30	H30A	0.9600
C30	H30B	0.9600	C30	H30C	0.9600

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C4	Zr1	C1	69.70(10)	C4	Zr1	C11	134.26(13)
C1	Zr1	C11	93.62(12)	C4	Zr1	C10	102.23(13)
C1	Zr1	C10	76.07(11)	C11	Zr1	C10	32.27(13)
C4	Zr1	C12	134.01(11)	C1	Zr1	C12	125.28(11)
C11	Zr1	C12	32.15(12)	C10	Zr1	C12	53.19(12)
C4	Zr1	C14	84.84(11)	C1	Zr1	C14	94.78(10)
C11	Zr1	C14	53.40(12)	C10	Zr1	C14	32.05(12)
C12	Zr1	C14	53.32(11)	C4	Zr1	C13	102.44(11)
C1	Zr1	C13	125.99(10)	C11	Zr1	C13	52.81(12)
C10	Zr1	C13	52.76(11)	C12	Zr1	C13	31.77(11)
C14	Zr1	C13	32.11(10)	C4	Zr1	C7	139.06(12)
C1	Zr1	C7	93.61(11)	C11	Zr1	C7	81.97(13)
C10	Zr1	C7	109.76(14)	C12	Zr1	C7	86.43(12)
C14	Zr1	C7	134.96(12)	C13	Zr1	C7	117.06(11)
C4	Zr1	C8	132.81(11)	C1	Zr1	C8	123.59(11)
C11	Zr1	C8	92.27(14)	C10	Zr1	C8	124.54(13)
C12	Zr1	C8	79.16(12)	C14	Zr1	C8	131.54(11)
C13	Zr1	C8	101.24(11)	C7	Zr1	C8	32.33(11)
C4	Zr1	C5	87.50(11)	C1	Zr1	C5	85.81(10)
C11	Zr1	C5	134.99(13)	C10	Zr1	C5	154.69(12)
C12	Zr1	C5	132.37(12)	C14	Zr1	C5	171.58(11)
C13	Zr1	C5	148.19(11)	C7	Zr1	C5	53.25(12)
C8	Zr1	C5	53.25(12)	C4	Zr1	C9	101.06(11)
C1	Zr1	C9	117.96(11)	C11	Zr1	C9	123.87(14)
C10	Zr1	C9	155.99(13)	C12	Zr1	C9	105.24(12)
C14	Zr1	C9	146.87(11)	C13	Zr1	C9	115.99(11)
C7	Zr1	C9	53.04(11)	C8	Zr1	C9	31.78(11)
C5	Zr1	C9	32.29(11)	C4	Zr1	C6	107.93(12)
C1	Zr1	C6	71.44(11)	C11	Zr1	C6	106.03(13)
C10	Zr1	C6	123.43(13)	C12	Zr1	C6	118.04(12)
C14	Zr1	C6	155.49(12)	C13	Zr1	C6	149.13(12)
C7	Zr1	C6	32.07(12)	C8	Zr1	C6	53.11(11)
C5	Zr1	C6	31.93(11)	C9	Zr1	C6	52.91(11)
C2	C1	C15	120.1(3)	C2	C1	Zr1	116.5(2)
C15	C1	Zr1	122.7(2)	C29	C28	C30	110.1(3)
C29	C28	P1	114.0(3)	C30	C28	P1	110.8(3)
C29	C28	H28A	107.2	C30	C28	H28A	107.2
P1	C28	H28A	107.2	C4	P1	C28	115.59(15)
C4	P1	C25	108.43(15)	C28	P1	C25	105.29(16)

C4	P1	Zr1	53.94(10)	C28	P1	Zr1	133.74(12)
C25	P1	Zr1	120.90(11)	C6	C5	C9	107.5(3)
C6	C5	Zr1	74.31(19)	C9	C5	Zr1	74.12(19)
C6	C5	H5A	125.8	C9	C5	H5A	125.8
Zr1	C5	H5A	125.8	C20	C19	C24	118.3(3)
C20	C19	C3	121.7(3)	C24	C19	C3	120.0(3)
C1	C2	C3	115.7(3)	C1	C2	C17	126.3(3)
C3	C2	C17	118.0(3)	C10	C14	C13	107.1(3)
C10	C14	Zr1	73.8(2)	C13	C14	Zr1	74.18(18)
C10	C14	H14A	126.0	C13	C14	H14A	126.0
Zr1	C14	H14A	126.0	C25	C27	H27A	109.5
C25	C27	H27B	109.5	H27A	C27	H27B	109.5
C25	C27	H27C	109.5	H27A	C27	H27C	109.5
H27B	C27	H27C	109.5	C23	C24	C19	120.7(3)
C23	C24	H24A	119.7	C19	C24	H24A	119.7
C3	C4	P1	146.6(3)	C3	C4	Zr1	120.6(2)
P1	C4	Zr1	87.36(12)	C4	C3	C2	114.7(3)
C4	C3	C19	123.6(3)	C2	C3	C19	121.7(3)
C17	C18	H18A	109.5	C17	C18	H18B	109.5
H18A	C18	H18B	109.5	C17	C18	H18C	109.5
H18A	C18	H18C	109.5	H18B	C18	H18C	109.5
C23	C22	C21	119.7(3)	C23	C22	H22A	120.2
C21	C22	H22A	120.2	C8	C9	C5	108.3(3)
C8	C9	Zr1	73.65(19)	C5	C9	Zr1	73.59(18)
C8	C9	H9A	125.6	C5	C9	H9A	125.6
Zr1	C9	H9A	125.6	C12	C13	C14	109.0(3)
C12	C13	Zr1	73.73(19)	C14	C13	Zr1	73.70(18)
C12	C13	H13A	125.3	C14	C13	H13A	125.3
Zr1	C13	H13A	125.3	C6	C7	C8	107.8(3)
C6	C7	Zr1	74.6(2)	C8	C7	Zr1	74.00(19)
C6	C7	H7A	125.7	C8	C7	H7A	125.7
Zr1	C7	H7A	125.7	C27	C25	C26	110.3(3)
C27	C25	P1	113.6(2)	C26	C25	P1	114.0(2)
C27	C25	H25A	106.1	C26	C25	H25A	106.1
P1	C25	H25A	106.1	C28	C29	H29A	109.5
C28	C29	H29B	109.5	H29A	C29	H29B	109.5
C28	C29	H29C	109.5	H29A	C29	H29C	109.5
H29B	C29	H29C	109.5	C25	C26	H26A	109.5
C25	C26	H26B	109.5	H26A	C26	H26B	109.5
C25	C26	H26C	109.5	H26A	C26	H26C	109.5
H26B	C26	H26C	109.5	C22	C23	C24	120.4(3)
C22	C23	H23A	119.8	C24	C23	H23A	119.8
C20	C21	C22	120.0(3)	C20	C21	H21A	120.0
C22	C21	H21A	120.0	C21	C20	C19	121.0(3)
C21	C20	H20A	119.5	C19	C20	H20A	119.5
C16	C15	C1	114.9(3)	C16	C15	H15A	108.5

C1	C15	H15A	108.5	C16	C15	H15B	108.5
C1	C15	H15B	108.5	H15A	C15	H15B	107.5
C2	C17	C18	113.9(3)	C2	C17	H17A	108.8
C18	C17	H17A	108.8	C2	C17	H17B	108.8
C18	C17	H17B	108.8	H17A	C17	H17B	107.7
C13	C12	C11	107.7(3)	C13	C12	Zr1	74.50(19)
C11	C12	Zr1	73.5(2)	C13	C12	H12A	125.7
C11	C12	H12A	125.7	Zr1	C12	H12A	125.7
C9	C8	C7	108.1(3)	C9	C8	Zr1	74.57(19)
C7	C8	Zr1	73.67(19)	C9	C8	H8A	125.6
C7	C8	H8A	125.6	Zr1	C8	H8A	125.6
C15	C16	H16A	109.5	C15	C16	H16B	109.5
H16A	C16	H16B	109.5	C15	C16	H16C	109.5
H16A	C16	H16C	109.5	H16B	C16	H16C	109.5
C12	C11	C10	107.9(3)	C12	C11	Zr1	74.4(2)
C10	C11	Zr1	74.3(2)	C12	C11	H11A	125.6
C10	C11	H11A	125.6	Zr1	C11	H11A	125.6
C14	C10	C11	108.3(3)	C14	C10	Zr1	74.15(19)
C11	C10	Zr1	73.5(2)	C14	C10	H10A	125.5
C11	C10	H10A	125.5	Zr1	C10	H10A	125.5
C5	C6	C7	108.4(3)	C5	C6	Zr1	73.76(19)
C7	C6	Zr1	73.33(19)	C5	C6	H6A	125.5
C7	C6	H6A	125.5	Zr1	C6	H6A	125.5
C28	C30	H30A	109.5	C28	C30	H30B	109.5
H30A	C30	H30B	109.5	C28	C30	H30C	109.5
H30A	C30	H30C	109.5	H30B	C30	H30C	109.5

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C4	Zr1	C1	C2	12.9(2)	C11	Zr1	C1	C2	149.2(2)
C10	Zr1	C1	C2	121.9(3)	C12	Zr1	C1	C2	143.1(2)
C14	Zr1	C1	C2	95.6(2)	C13	Zr1	C1	C2	103.8(2)
C7	Zr1	C1	C2	-128.7(2)	C8	Zr1	C1	C2	-115.7(2)
C5	Zr1	C1	C2	-76.0(2)	C9	Zr1	C1	C2	-79.1(3)
C6	Zr1	C1	C2	-105.1(2)	C4	Zr1	C1	C15	-177.2(3)
C11	Zr1	C1	C15	-41.0(3)	C10	Zr1	C1	C15	-68.3(2)
C12	Zr1	C1	C15	-47.0(3)	C14	Zr1	C1	C15	-94.5(2)
C13	Zr1	C1	C15	-86.4(3)	C7	Zr1	C1	C15	41.2(2)
C8	Zr1	C1	C15	54.2(3)	C5	Zr1	C1	C15	93.9(2)
C9	Zr1	C1	C15	90.8(2)	C6	Zr1	C1	C15	64.7(2)
C29	C28	P1	C4	-40.1(3)	C30	C28	P1	C4	-165.1(3)
C29	C28	P1	C25	-159.8(3)	C30	C28	P1	C25	75.3(3)
C29	C28	P1	Zr1	23.4(4)	C30	C28	P1	Zr1	-101.5(3)
C1	Zr1	P1	C4	4.16(15)	C11	Zr1	P1	C4	-110.2(2)
C10	Zr1	P1	C4	-78.52(16)	C12	Zr1	P1	C4	-136.30(16)
C14	Zr1	P1	C4	-88.97(14)	C13	Zr1	P1	C4	-121.25(15)
C7	Zr1	P1	C4	118.39(17)	C8	Zr1	P1	C4	139.30(15)
C5	Zr1	P1	C4	88.96(15)	C9	Zr1	P1	C4	120.72(15)
C6	Zr1	P1	C4	82.62(15)	C4	Zr1	P1	C28	-92.5(2)
C1	Zr1	P1	C28	-88.30(18)	C11	Zr1	P1	C28	157.3(2)
C10	Zr1	P1	C28	-170.97(19)	C12	Zr1	P1	C28	131.25(19)
C14	Zr1	P1	C28	178.57(18)	C13	Zr1	P1	C28	146.29(18)
C7	Zr1	P1	C28	25.9(2)	C8	Zr1	P1	C28	46.84(19)
C5	Zr1	P1	C28	-3.50(18)	C9	Zr1	P1	C28	28.27(19)
C6	Zr1	P1	C28	-9.84(19)	C4	Zr1	P1	C25	91.15(17)
C1	Zr1	P1	C25	95.31(14)	C11	Zr1	P1	C25	-19.1(2)
C10	Zr1	P1	C25	12.63(16)	C12	Zr1	P1	C25	-45.15(15)
C14	Zr1	P1	C25	2.18(14)	C13	Zr1	P1	C25	-30.10(14)
C7	Zr1	P1	C25	-150.46(17)	C8	Zr1	P1	C25	-129.55(15)
C5	Zr1	P1	C25	-179.89(15)	C9	Zr1	P1	C25	-148.13(15)
C6	Zr1	P1	C25	173.77(15)	C4	Zr1	C5	C6	-130.7(2)
C1	Zr1	C5	C6	-60.9(2)	C11	Zr1	C5	C6	30.0(3)
C10	Zr1	C5	C6	-16.9(4)	C12	Zr1	C5	C6	74.9(3)
C14	Zr1	C5	C6	-155.3(7)	C13	Zr1	C5	C6	119.5(3)
C7	Zr1	C5	C6	36.7(2)	C8	Zr1	C5	C6	77.4(2)
C9	Zr1	C5	C6	113.9(3)	C4	Zr1	C5	C9	115.4(2)
C1	Zr1	C5	C9	-174.8(2)	C11	Zr1	C5	C9	-83.9(3)
C10	Zr1	C5	C9	-130.8(3)	C12	Zr1	C5	C9	-39.0(3)
C14	Zr1	C5	C9	90.9(8)	C13	Zr1	C5	C9	5.6(3)

C7	Zr1	C5	C9	-77.1(2)	C8	Zr1	C5	C9	-36.5(2)
C6	Zr1	C5	C9	-113.9(3)	C15	C1	C2	C3	180.0(2)
Zr1	C1	C2	C3	-9.9(3)	C15	C1	C2	C17	0.8(5)
Zr1	C1	C2	C17	171.0(2)	C4	Zr1	C14	C10	123.0(2)
C1	Zr1	C14	C10	53.9(2)	C11	Zr1	C14	C10	-37.0(2)
C12	Zr1	C14	C10	-77.4(2)	C13	Zr1	C14	C10	-113.6(3)
C7	Zr1	C14	C10	-46.0(3)	C8	Zr1	C14	C10	-90.7(2)
C5	Zr1	C14	C10	147.6(7)	C9	Zr1	C14	C10	-134.6(3)
C6	Zr1	C14	C10	-0.1(4)	C4	Zr1	C14	C13	-123.4(2)
C1	Zr1	C14	C13	167.5(2)	C11	Zr1	C14	C13	76.5(2)
C10	Zr1	C14	C13	113.6(3)	C12	Zr1	C14	C13	36.17(19)
C7	Zr1	C14	C13	67.6(3)	C8	Zr1	C14	C13	22.8(3)
C5	Zr1	C14	C13	-98.8(7)	C9	Zr1	C14	C13	-21.1(3)
C6	Zr1	C14	C13	113.4(3)	C20	C19	C24	C23	-0.1(4)
C3	C19	C24	C23	-179.8(3)	C28	P1	C4	C3	-21.8(5)
C25	P1	C4	C3	96.1(5)	Zr1	P1	C4	C3	-148.7(5)
C28	P1	C4	Zr1	126.84(15)	C25	P1	C4	Zr1	-115.27(13)
C1	Zr1	C4	C3	-15.2(2)	C11	Zr1	C4	C3	-89.8(3)
C10	Zr1	C4	C3	-85.2(3)	C12	Zr1	C4	C3	-135.1(2)
C14	Zr1	C4	C3	-112.3(3)	C13	Zr1	C4	C3	-139.3(2)
C7	Zr1	C4	C3	55.9(3)	C8	Zr1	C4	C3	102.3(3)
C5	Zr1	C4	C3	71.2(3)	C9	Zr1	C4	C3	100.7(3)
C6	Zr1	C4	C3	46.3(3)	C1	Zr1	C4	P1	-175.79(15)
C11	Zr1	C4	P1	109.67(17)	C10	Zr1	C4	P1	114.26(13)
C12	Zr1	C4	P1	64.28(19)	C14	Zr1	C4	P1	87.17(12)
C13	Zr1	C4	P1	60.15(13)	C7	Zr1	C4	P1	-104.69(17)
C8	Zr1	C4	P1	-58.31(19)	C5	Zr1	C4	P1	-89.33(13)
C9	Zr1	C4	P1	-59.87(14)	C6	Zr1	C4	P1	-114.24(12)
P1	C4	C3	C2	158.5(4)	Zr1	C4	C3	C2	15.6(4)
P1	C4	C3	C19	-20.7(6)	Zr1	C4	C3	C19	-163.6(2)
C1	C2	C3	C4	-2.9(4)	C17	C2	C3	C4	176.3(3)
C1	C2	C3	C19	176.2(3)	C17	C2	C3	C19	-4.5(4)
C20	C19	C3	C4	111.8(4)	C24	C19	C3	C4	-68.5(4)
C20	C19	C3	C2	-67.3(4)	C24	C19	C3	C2	112.4(3)
C6	C5	C9	C8	-1.4(4)	Zr1	C5	C9	C8	66.0(2)
C6	C5	C9	Zr1	-67.4(2)	C4	Zr1	C9	C8	177.8(2)
C1	Zr1	C9	C8	-109.4(2)	C11	Zr1	C9	C8	6.8(3)
C10	Zr1	C9	C8	12.0(4)	C12	Zr1	C9	C8	35.9(2)
C14	Zr1	C9	C8	80.2(3)	C13	Zr1	C9	C8	68.0(2)
C7	Zr1	C9	C8	-37.5(2)	C5	Zr1	C9	C8	-115.3(3)
C6	Zr1	C9	C8	-78.0(2)	C4	Zr1	C9	C5	-66.9(2)
C1	Zr1	C9	C5	5.9(3)	C11	Zr1	C9	C5	122.1(2)
C10	Zr1	C9	C5	127.3(3)	C12	Zr1	C9	C5	151.2(2)
C14	Zr1	C9	C5	-164.5(2)	C13	Zr1	C9	C5	-176.7(2)
C7	Zr1	C9	C5	77.8(2)	C8	Zr1	C9	C5	115.3(3)
C6	Zr1	C9	C5	37.3(2)	C10	C14	C13	C12	1.2(4)

Zr1	C14	C13	C12	-65.8(2)	C10	C14	C13	Zr1	67.0(2)
C4	Zr1	C13	C12	174.3(2)	C1	Zr1	C13	C12	100.5(2)
C11	Zr1	C13	C12	37.5(2)	C10	Zr1	C13	C12	78.3(2)
C14	Zr1	C13	C12	116.0(3)	C7	Zr1	C13	C12	-16.7(2)
C8	Zr1	C13	C12	-46.8(2)	C5	Zr1	C13	C12	-79.9(3)
C9	Zr1	C13	C12	-76.6(2)	C6	Zr1	C13	C12	-16.1(3)
C4	Zr1	C13	C14	58.3(2)	C1	Zr1	C13	C14	-15.5(3)
C11	Zr1	C13	C14	-78.5(2)	C10	Zr1	C13	C14	-37.7(2)
C12	Zr1	C13	C14	-116.0(3)	C7	Zr1	C13	C14	-132.7(2)
C8	Zr1	C13	C14	-162.8(2)	C5	Zr1	C13	C14	164.1(2)
C9	Zr1	C13	C14	167.4(2)	C6	Zr1	C13	C14	-132.1(2)
C4	Zr1	C7	C6	-17.3(3)	C1	Zr1	C7	C6	45.5(2)
C11	Zr1	C7	C6	138.6(2)	C10	Zr1	C7	C6	121.9(2)
C12	Zr1	C7	C6	170.6(2)	C14	Zr1	C7	C6	145.9(2)
C13	Zr1	C7	C6	179.4(2)	C8	Zr1	C7	C6	-114.1(3)
C5	Zr1	C7	C6	-36.6(2)	C9	Zr1	C7	C6	-77.3(2)
C4	Zr1	C7	C8	96.8(3)	C1	Zr1	C7	C8	159.5(2)
C11	Zr1	C7	C8	-107.3(2)	C10	Zr1	C7	C8	-124.0(2)
C12	Zr1	C7	C8	-75.3(2)	C14	Zr1	C7	C8	-100.0(2)
C13	Zr1	C7	C8	-66.6(2)	C5	Zr1	C7	C8	77.5(2)
C9	Zr1	C7	C8	36.8(2)	C6	Zr1	C7	C8	114.1(3)
C4	P1	C25	C27	-82.8(3)	C28	P1	C25	C27	41.5(3)
Zr1	P1	C25	C27	-141.2(2)	C4	P1	C25	C26	149.8(2)
C28	P1	C25	C26	-86.0(3)	Zr1	P1	C25	C26	91.3(3)
C21	C22	C23	C24	0.6(5)	C19	C24	C23	C22	-0.7(5)
C23	C22	C21	C20	0.3(5)	C22	C21	C20	C19	-1.1(5)
C24	C19	C20	C21	1.0(4)	C3	C19	C20	C21	-179.3(3)
C2	C1	C15	C16	-71.3(4)	Zr1	C1	C15	C16	119.2(3)
C1	C2	C17	C18	109.0(4)	C3	C2	C17	C18	-70.2(4)
C14	C13	C12	C11	-0.7(4)	Zr1	C13	C12	C11	-66.5(2)
C14	C13	C12	Zr1	65.8(2)	C4	Zr1	C12	C13	-7.7(3)
C1	Zr1	C12	C13	-103.0(2)	C11	Zr1	C12	C13	-114.3(3)
C10	Zr1	C12	C13	-76.9(2)	C14	Zr1	C12	C13	-36.57(19)
C7	Zr1	C12	C13	165.1(2)	C8	Zr1	C12	C13	133.3(2)
C5	Zr1	C12	C13	135.4(2)	C9	Zr1	C12	C13	115.0(2)
C6	Zr1	C12	C13	170.73(19)	C4	Zr1	C12	C11	106.6(3)
C1	Zr1	C12	C11	11.3(3)	C10	Zr1	C12	C11	37.4(2)
C14	Zr1	C12	C11	77.8(3)	C13	Zr1	C12	C11	114.3(3)
C7	Zr1	C12	C11	-80.6(2)	C8	Zr1	C12	C11	-112.4(3)
C5	Zr1	C12	C11	-110.3(3)	C9	Zr1	C12	C11	-130.7(2)
C6	Zr1	C12	C11	-75.0(3)	C5	C9	C8	C7	0.6(4)
Zr1	C9	C8	C7	66.6(2)	C5	C9	C8	Zr1	-66.0(2)
C6	C7	C8	C9	0.3(4)	Zr1	C7	C8	C9	-67.2(2)
C6	C7	C8	Zr1	67.6(2)	C4	Zr1	C8	C9	-2.9(3)
C1	Zr1	C8	C9	89.8(2)	C11	Zr1	C8	C9	-174.3(2)
C10	Zr1	C8	C9	-174.1(2)	C12	Zr1	C8	C9	-144.8(2)

C14	Zr1	C8	C9	-134.0(2)	C13	Zr1	C8	C9	-121.8(2)
C7	Zr1	C8	C9	114.6(3)	C5	Zr1	C8	C9	37.1(2)
C6	Zr1	C8	C9	77.3(2)	C4	Zr1	C8	C7	-117.5(2)
C1	Zr1	C8	C7	-24.8(3)	C11	Zr1	C8	C7	71.1(2)
C10	Zr1	C8	C7	71.3(3)	C12	Zr1	C8	C7	100.6(2)
C14	Zr1	C8	C7	111.4(2)	C13	Zr1	C8	C7	123.6(2)
C5	Zr1	C8	C7	-77.5(2)	C9	Zr1	C8	C7	-114.6(3)
C6	Zr1	C8	C7	-37.3(2)	C13	C12	C11	C10	-0.1(4)
Zr1	C12	C11	C10	-67.3(2)	C13	C12	C11	Zr1	67.2(2)
C4	Zr1	C11	C12	-105.8(3)	C1	Zr1	C11	C12	-170.8(2)
C10	Zr1	C11	C12	-114.3(3)	C14	Zr1	C11	C12	-77.5(2)
C13	Zr1	C11	C12	-37.0(2)	C7	Zr1	C11	C12	96.1(2)
C8	Zr1	C11	C12	65.4(2)	C5	Zr1	C11	C12	101.5(3)
C9	Zr1	C11	C12	61.8(3)	C6	Zr1	C11	C12	117.5(2)
C4	Zr1	C11	C10	8.4(3)	C1	Zr1	C11	C10	-56.5(2)
C12	Zr1	C11	C10	114.3(3)	C14	Zr1	C11	C10	36.8(2)
C13	Zr1	C11	C10	77.2(2)	C7	Zr1	C11	C10	-149.6(2)
C8	Zr1	C11	C10	179.6(2)	C5	Zr1	C11	C10	-144.2(2)
C9	Zr1	C11	C10	176.0(2)	C6	Zr1	C11	C10	-128.2(2)
C13	C14	C10	C11	-1.2(4)	Zr1	C14	C10	C11	66.1(2)
C13	C14	C10	Zr1	-67.3(2)	C12	C11	C10	C14	0.8(4)
Zr1	C11	C10	C14	-66.5(2)	C12	C11	C10	Zr1	67.3(3)
C4	Zr1	C10	C14	-58.7(2)	C1	Zr1	C10	C14	-123.9(2)
C11	Zr1	C10	C14	115.1(3)	C12	Zr1	C10	C14	77.8(2)
C13	Zr1	C10	C14	37.74(19)	C7	Zr1	C10	C14	147.3(2)
C8	Zr1	C10	C14	114.7(2)	C5	Zr1	C10	C14	-169.4(2)
C9	Zr1	C10	C14	107.0(3)	C6	Zr1	C10	C14	179.93(19)
C4	Zr1	C10	C11	-173.8(2)	C1	Zr1	C10	C11	121.0(2)
C12	Zr1	C10	C11	-37.3(2)	C14	Zr1	C10	C11	-115.1(3)
C13	Zr1	C10	C11	-77.4(2)	C7	Zr1	C10	C11	32.1(3)
C8	Zr1	C10	C11	-0.5(3)	C5	Zr1	C10	C11	75.4(4)
C9	Zr1	C10	C11	-8.1(4)	C6	Zr1	C10	C11	64.8(3)
C9	C5	C6	C7	1.6(4)	Zr1	C5	C6	C7	-65.7(2)
C9	C5	C6	Zr1	67.3(2)	C8	C7	C6	C5	-1.2(4)
Zr1	C7	C6	C5	66.0(2)	C8	C7	C6	Zr1	-67.1(2)
C4	Zr1	C6	C5	52.7(2)	C1	Zr1	C6	C5	113.1(2)
C11	Zr1	C6	C5	-158.4(2)	C10	Zr1	C6	C5	171.4(2)
C12	Zr1	C6	C5	-126.1(2)	C14	Zr1	C6	C5	171.5(2)
C13	Zr1	C6	C5	-116.6(3)	C7	Zr1	C6	C5	-115.5(3)
C8	Zr1	C6	C5	-77.9(2)	C9	Zr1	C6	C5	-37.8(2)
C4	Zr1	C6	C7	168.2(2)	C1	Zr1	C6	C7	-131.4(2)
C11	Zr1	C6	C7	-42.9(2)	C10	Zr1	C6	C7	-73.1(2)
C12	Zr1	C6	C7	-10.6(3)	C14	Zr1	C6	C7	-73.0(3)
C13	Zr1	C6	C7	-1.1(3)	C8	Zr1	C6	C7	37.6(2)
C5	Zr1	C6	C7	115.5(3)	C9	Zr1	C6	C7	77.7(2)

X-Ray Structural Data for 10:

Data Collection

A fragment of a red block-like crystal of C36 H35 P Zr having approximate dimensions of .15 x .15 x .1 mm was mounted on a glass fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker P4 [10] CCD area detector with graphite monochromated MoKradiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 1357 centered reflections with I > $10\sigma(I)$ in the range $3.44 < \theta < 19.3^o$ corresponded to a primitive Monoclinic cell with dimensions:

a = 29.784(6) Å	$\alpha = 90^o$
b = 9.968(2) Å	$\beta = 96.40(3)^o$
c = 19.424(4) Å	$\gamma = 90^o$
V = 8876(1) Å^3	

For Z = 8 and F.W. = 589.83, the calculated density is 1.367 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

P2(1)/c

The data were collected at a temperature of 163(2) K. Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3^o counted for a total of 30 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[11] to a maximum θ value of 20.90^o. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP[12]. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS[13]. (Tmax = 0.96, Tmin = 0.90). Of the 14794 reflections that were collected, 5719 were unique (R_{int} = 0.0766); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the

rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 5719 reflections (all data) and 685 variable parameters and converged (largest parameter shift was 0.001 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0497 \text{ for 3598 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.0965$$

The standard deviation of an observation of unit weight[4] was 0.983. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.784 and -0.399 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the SHELXTL[9] crystallographic software package of Bruker Analytical X-ray Systems Inc.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C36 H35 P Zr
Formula Weight	589.83
Crystal Color, Habit	red, block
Crystal Dimensions	.15 x .15 x .1 mm
Crystal System	Monoclinic
Lattice Type	primitive
Lattice Parameters	a = 29.784(6) Å b = 9.968(2) Å c = 19.424(4) Å α= 90 ° β= 96.40(3) ° γ = 90° V = 5731(2) $Å^3$
Space Group	P2(1)/c
Z value	8
D_{calc}	1.367 g/cm^3

F_{000}	2448
μ(MoK)	0.46 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker P4
Radiation	MoK(λ = 0.71073 Å) graphite monochromated
Detector Position	60.00 mm
Exposure Time	30 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
θ_{max}	20.90°
No. of Reflections Measured	Total: 14794 Unique: 5719 (R_{int} = 0.0766)
Corrections	Lorentz-polarization Absorption (Tmax = 0.96, Tmin = 0.90)

C. Structure Solution and Refinement

Structure Solution	direct (SHELXS-97 (Sheldrick, 1990))
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|F_o\|^2 - \|F_c\|^2)^2$
Least Squares Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (qP)^2 + 0.000P]$ where $P = [F_o^2 + 2F_c^2]/3$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.00σ(I))	3598
No. Variables	685
Residuals: R; wR_2; Rall	0.0497; 0.0965; 0.1017
Goodness of Fit Indicator	0.983
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.784 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.399 $e^-/Å^3$

Table 1. Atomic coordinates and U_{iso}/U_{eq} and occupancy

atom	x	y	z	U_{eq}	Occupancy
Zr1	0.1148(1)	0.6652(1)	0.3370(1)	0.028(1)	1
P1	0.1655(1)	0.7692(2)	0.5146(1)	0.029(1)	1
C1	0.0876(2)	0.4630(7)	0.3606(4)	0.029(2)	1
C2	0.0972(2)	0.4337(7)	0.4280(4)	0.029(2)	1
C3	0.1253(2)	0.5285(7)	0.4755(3)	0.020(2)	1
C4	0.1333(2)	0.6568(7)	0.4539(3)	0.023(2)	1
C5	0.0763(3)	0.8817(8)	0.3074(5)	0.043(2)	1
C6	0.0635(3)	0.8002(9)	0.2517(5)	0.045(2)	1
C7	0.0371(2)	0.6994(8)	0.2733(5)	0.041(2)	1
C8	0.0328(2)	0.7169(10)	0.3430(5)	0.049(3)	1
C9	0.0574(3)	0.8319(9)	0.3648(5)	0.047(2)	1
C10	0.1563(2)	0.5465(9)	0.2501(5)	0.043(2)	1
C11	0.1780(2)	0.5114(8)	0.3153(4)	0.033(2)	1
C12	0.1979(2)	0.6267(8)	0.3449(4)	0.034(2)	1
C13	0.1886(2)	0.7336(8)	0.2993(4)	0.039(2)	1
C14	0.1636(2)	0.6823(9)	0.2400(4)	0.043(2)	1
C15	0.0591(2)	0.3698(7)	0.3114(4)	0.036(2)	1
C16	0.0853(2)	0.2551(8)	0.2848(4)	0.054(2)	1
C17	0.0783(2)	0.3127(6)	0.4625(4)	0.031(2)	1
C18	0.0385(2)	0.3494(7)	0.5020(4)	0.041(2)	1
C19	0.1446(2)	0.4732(6)	0.5435(4)	0.024(2)	1
C20	0.1781(2)	0.3733(7)	0.5442(4)	0.032(2)	1
C21	0.1980(2)	0.3196(7)	0.6044(5)	0.035(2)	1
C22	0.1852(2)	0.3619(8)	0.6671(4)	0.040(2)	1
C23	0.1530(3)	0.4594(8)	0.6688(4)	0.044(2)	1
C24	0.1330(2)	0.5129(7)	0.6067(4)	0.035(2)	1
C25	0.0771(2)	0.8231(7)	0.5488(4)	0.032(2)	1
C26	0.1204(2)	0.8723(7)	0.5458(4)	0.030(2)	1
C27	0.1302(2)	0.9990(8)	0.5715(3)	0.029(2)	1
C28	0.0983(3)	1.0767(7)	0.5992(4)	0.036(2)	1
C29	0.0557(3)	1.0249(8)	0.6024(4)	0.040(2)	1
C30	0.0453(2)	0.9002(8)	0.5779(4)	0.037(2)	1
C31	0.1909(2)	0.8903(7)	0.4596(4)	0.030(2)	1
C32	0.2363(2)	0.8761(7)	0.4527(4)	0.038(2)	1
C33	0.2586(3)	0.9619(9)	0.4112(4)	0.044(2)	1
C34	0.2365(3)	1.0659(9)	0.3784(4)	0.047(2)	1
C35	0.1912(3)	1.0853(8)	0.3843(4)	0.046(2)	1
C36	0.1686(2)	0.9976(8)	0.4236(4)	0.037(2)	1
Zr2	0.3714(1)	0.4925(1)	0.5155(1)	0.032(1)	1
P2	0.3762(1)	0.3072(2)	0.6867(1)	0.032(1)	1

C101	0.4191(2)	0.3691(7)	0.4608(4)	0.033(2)	1
C102	0.4336(2)	0.2667(8)	0.5018(4)	0.031(2)	1
C103	0.4210(2)	0.2578(7)	0.5743(4)	0.028(2)	1
C104	0.3878(2)	0.3342(7)	0.5981(4)	0.026(2)	1
C105	0.2883(2)	0.5169(9)	0.4949(4)	0.041(2)	1
C106	0.3046(2)	0.5649(8)	0.4339(4)	0.044(2)	1
C107	0.3226(3)	0.4569(10)	0.4022(5)	0.051(2)	1
C108	0.3181(2)	0.3418(9)	0.4412(5)	0.051(2)	1
C109	0.2958(2)	0.3779(9)	0.4986(4)	0.043(2)	1
C110	0.4104(3)	0.7097(8)	0.4960(5)	0.052(3)	1
C111	0.4415(3)	0.6342(8)	0.5379(6)	0.050(2)	1
C112	0.4253(3)	0.6166(8)	0.6009(5)	0.050(2)	1
C113	0.3838(3)	0.6849(8)	0.5991(5)	0.047(2)	1
C115	0.4292(3)	0.3701(8)	0.3859(5)	0.056(3)	1
C116	0.4351(3)	0.5060(10)	0.3585(5)	0.088(3)	1
C117	0.4590(2)	0.1485(7)	0.4758(4)	0.045(2)	1
C118	0.4269(3)	0.0447(8)	0.4407(4)	0.060(3)	1
C119	0.4483(2)	0.1616(7)	0.6221(4)	0.026(2)	1
C120	0.4393(2)	0.0278(8)	0.6285(4)	0.037(2)	1
C121	0.4675(3)	-0.0546(8)	0.6709(4)	0.039(2)	1
C122	0.5053(3)	-0.0025(9)	0.7083(4)	0.041(2)	1
C123	0.5147(2)	0.1298(9)	0.7039(4)	0.043(2)	1
C124	0.4869(2)	0.2113(7)	0.6614(4)	0.036(2)	1
C125	0.3293(2)	0.1878(7)	0.6749(4)	0.031(2)	1
C126	0.3027(2)	0.1723(8)	0.7287(4)	0.041(2)	1
C127	0.2691(3)	0.0784(9)	0.7256(5)	0.049(2)	1
C128	0.2606(2)	-0.0041(8)	0.6689(5)	0.048(2)	1
C129	0.2868(2)	0.0087(8)	0.6148(4)	0.044(2)	1
C130	0.3210(2)	0.1050(8)	0.6183(4)	0.039(2)	1
C131	0.3451(2)	0.4569(7)	0.7099(4)	0.031(2)	1
C132	0.3656(2)	0.5386(8)	0.7611(4)	0.041(2)	1
C133	0.3457(3)	0.6558(8)	0.7815(4)	0.049(2)	1
C134	0.3038(3)	0.6913(8)	0.7510(5)	0.048(2)	1
C135	0.2816(3)	0.6078(9)	0.7006(5)	0.047(2)	1
C136	0.3020(2)	0.4937(8)	0.6802(4)	0.033(2)	1
C114	0.3748(3)	0.7414(8)	0.5336(5)	0.050(2)	1

U_{eq} is defined as one third of the orthogonalized U_{ij} tensor

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr1	0.025(1)	0.037(1)	0.023(1)	0.002(1)	0.004(1)	0.001(1)
P1	0.032(1)	0.029(1)	0.026(2)	-0.001(1)	0.004(1)	-0.002(1)
C1	0.020(4)	0.040(5)	0.028(6)	-0.006(4)	0.003(4)	0.004(3)
C2	0.026(4)	0.028(5)	0.033(6)	0.006(4)	0.002(4)	0.004(4)
C3	0.017(4)	0.028(5)	0.016(5)	-0.001(4)	0.002(3)	0.004(3)
C4	0.017(4)	0.032(5)	0.022(5)	-0.011(4)	0.006(3)	0.008(3)
C5	0.047(5)	0.029(5)	0.054(7)	0.011(5)	0.007(5)	0.003(4)
C6	0.045(5)	0.063(7)	0.027(6)	0.016(5)	0.004(4)	0.014(5)
C7	0.021(5)	0.038(6)	0.061(8)	0.008(5)	-0.012(4)	0.002(4)
C8	0.027(5)	0.077(8)	0.045(8)	0.035(6)	0.012(5)	0.024(5)
C9	0.045(5)	0.046(6)	0.049(7)	-0.017(5)	-0.002(5)	0.028(5)
C10	0.038(5)	0.057(7)	0.036(7)	-0.019(5)	0.019(5)	-0.009(4)
C11	0.029(4)	0.044(5)	0.029(6)	-0.001(5)	0.017(4)	0.005(4)
C12	0.016(4)	0.049(6)	0.039(6)	-0.003(5)	0.004(4)	0.005(4)
C13	0.036(5)	0.047(6)	0.036(7)	-0.015(5)	0.010(4)	-0.016(4)
C14	0.037(5)	0.074(7)	0.021(6)	0.003(5)	0.017(4)	-0.005(5)
C15	0.036(5)	0.040(5)	0.030(6)	0.000(4)	-0.007(4)	0.001(4)
C16	0.057(6)	0.045(6)	0.058(7)	-0.024(5)	0.006(5)	-0.009(4)
C17	0.027(4)	0.033(5)	0.032(5)	-0.001(4)	-0.002(4)	-0.005(4)
C18	0.036(5)	0.043(5)	0.047(6)	0.007(4)	0.013(4)	-0.007(4)
C19	0.039(5)	0.011(4)	0.022(6)	-0.002(4)	0.002(4)	-0.001(4)
C20	0.035(5)	0.032(5)	0.031(6)	0.001(4)	0.009(4)	0.002(4)
C21	0.029(5)	0.037(5)	0.038(7)	0.006(5)	0.005(4)	-0.001(4)
C22	0.042(5)	0.049(6)	0.026(6)	0.009(4)	-0.009(4)	-0.002(4)
C23	0.049(5)	0.051(6)	0.033(7)	0.001(5)	0.013(5)	-0.001(5)
C24	0.046(5)	0.028(5)	0.029(6)	-0.001(4)	0.005(4)	0.009(4)
C25	0.029(5)	0.027(5)	0.038(6)	0.001(4)	0.004(4)	-0.002(4)
C26	0.038(5)	0.026(5)	0.025(5)	0.003(4)	0.002(4)	0.003(4)
C27	0.031(4)	0.039(5)	0.018(5)	0.005(4)	0.006(4)	0.003(4)
C28	0.056(6)	0.026(5)	0.027(6)	0.002(4)	0.003(4)	0.002(5)
C29	0.048(6)	0.043(6)	0.029(6)	0.007(4)	0.008(4)	0.017(5)
C30	0.029(5)	0.038(6)	0.044(6)	0.001(4)	0.008(4)	0.008(4)
C31	0.034(5)	0.034(5)	0.023(5)	-0.007(4)	0.003(4)	0.001(4)
C32	0.027(5)	0.036(5)	0.049(6)	-0.001(4)	0.002(4)	0.001(4)
C33	0.030(5)	0.057(6)	0.045(6)	-0.007(5)	0.007(4)	-0.017(5)
C34	0.055(6)	0.052(6)	0.034(6)	0.003(5)	0.004(5)	-0.029(5)
C35	0.051(6)	0.043(6)	0.043(7)	0.009(4)	0.000(5)	-0.009(5)
C36	0.030(4)	0.038(5)	0.042(6)	0.004(5)	0.004(4)	-0.010(4)
Zr2	0.030(1)	0.037(1)	0.029(1)	0.002(1)	0.005(1)	-0.002(1)
P2	0.030(1)	0.040(1)	0.026(2)	-0.003(1)	0.006(1)	-0.002(1)

C101	0.037(5)	0.041(5)	0.022(6)	0.012(4)	0.013(4)	-0.006(4)
C102	0.017(4)	0.044(5)	0.034(6)	-0.014(5)	0.010(4)	-0.001(4)
C103	0.021(4)	0.037(5)	0.025(6)	-0.001(4)	0.002(4)	-0.006(4)
C104	0.022(4)	0.028(4)	0.028(5)	-0.003(4)	0.005(4)	-0.005(4)
C105	0.024(5)	0.065(7)	0.033(6)	0.003(5)	-0.003(4)	0.002(4)
C106	0.033(5)	0.056(6)	0.043(7)	0.009(5)	0.004(5)	0.016(4)
C107	0.044(5)	0.081(7)	0.026(6)	-0.003(6)	-0.013(4)	0.013(5)
C108	0.035(5)	0.057(7)	0.057(7)	-0.019(6)	-0.017(5)	0.001(5)
C109	0.024(5)	0.055(7)	0.049(7)	-0.008(5)	0.000(4)	-0.008(4)
C110	0.081(7)	0.032(6)	0.050(7)	0.001(5)	0.034(6)	-0.015(5)
C111	0.038(5)	0.047(6)	0.068(8)	-0.009(5)	0.012(6)	-0.015(5)
C112	0.050(6)	0.044(6)	0.050(8)	-0.004(5)	-0.017(5)	-0.013(5)
C113	0.063(7)	0.039(6)	0.041(7)	-0.018(5)	0.019(5)	-0.015(5)
C115	0.042(5)	0.055(6)	0.070(8)	0.027(5)	0.009(5)	0.017(4)
C116	0.109(8)	0.091(9)	0.074(8)	0.000(7)	0.052(7)	-0.005(7)
C117	0.049(5)	0.053(6)	0.034(6)	0.007(5)	0.014(4)	0.019(5)
C118	0.087(7)	0.053(6)	0.045(7)	-0.010(5)	0.025(5)	-0.007(5)
C119	0.031(5)	0.027(5)	0.021(5)	-0.002(4)	0.006(4)	0.003(4)
C120	0.035(5)	0.041(6)	0.035(6)	-0.004(4)	0.007(4)	-0.001(4)
C121	0.046(5)	0.033(5)	0.039(6)	-0.001(5)	0.015(5)	-0.002(5)
C122	0.052(6)	0.047(6)	0.024(6)	-0.001(5)	0.003(4)	0.006(5)
C123	0.038(5)	0.050(6)	0.040(6)	-0.013(5)	-0.004(4)	0.008(5)
C124	0.035(5)	0.034(5)	0.038(6)	-0.012(4)	0.001(4)	0.003(4)
C125	0.027(4)	0.040(5)	0.027(6)	0.007(4)	0.010(4)	0.004(4)
C126	0.038(5)	0.052(6)	0.034(6)	0.009(4)	0.006(4)	-0.001(5)
C127	0.035(6)	0.053(6)	0.060(8)	0.018(5)	0.011(5)	-0.001(5)
C128	0.029(5)	0.046(6)	0.067(8)	0.019(6)	0.002(5)	-0.007(4)
C129	0.040(5)	0.042(5)	0.050(7)	-0.001(5)	-0.001(5)	-0.004(5)
C130	0.031(5)	0.051(6)	0.035(6)	0.004(5)	0.008(4)	-0.002(4)
C131	0.022(5)	0.045(5)	0.027(6)	0.006(4)	0.006(4)	-0.002(4)
C132	0.039(5)	0.056(6)	0.030(6)	-0.002(5)	0.010(4)	0.007(5)
C133	0.062(6)	0.051(6)	0.035(6)	-0.018(5)	0.010(5)	-0.006(5)
C134	0.050(6)	0.036(6)	0.062(7)	-0.004(5)	0.028(5)	0.009(5)
C135	0.037(5)	0.051(6)	0.056(7)	0.004(5)	0.018(5)	0.008(5)
C136	0.031(5)	0.045(5)	0.024(5)	-0.005(4)	0.001(4)	0.002(4)
C114	0.063(6)	0.036(5)	0.049(8)	0.001(5)	-0.001(6)	0.002(4)

The general temperature factor expression:

$\exp(-2\Pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}\,hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Zr1	C1	2.239(7)	Zr1	C4	2.278(7)
Zr1	C5	2.481(7)	Zr1	C9	2.487(7)
Zr1	C13	2.488(7)	Zr1	C12	2.493(6)
Zr1	C11	2.499(7)	Zr1	C10	2.500(7)
Zr1	C14	2.510(7)	Zr1	C8	2.512(7)
Zr1	C6	2.515(7)	Zr1	C7	2.523(7)
P1	C4	1.819(7)	P1	C31	1.831(7)
P1	C26	1.846(7)	C1	C2	1.341(9)
C1	C15	1.522(9)	C2	C3	1.509(9)
C2	C17	1.518(9)	C3	C4	1.375(8)
C3	C19	1.486(9)	C5	C6	1.373(10)
C5	C9	1.396(10)	C5	H5A	0.9800
C6	C7	1.370(9)	C6	H6A	0.9800
C7	C8	1.386(10)	C7	H7A	0.9800
C8	C9	1.401(10)	C8	H8A	0.9800
C9	H9A	0.9800	C10	C14	1.388(10)
C10	C11	1.401(10)	C10	H10A	0.9800
C11	C12	1.388(9)	C11	H11A	0.9800
C12	C13	1.394(10)	C12	H12A	0.9800
C13	C14	1.397(9)	C13	H13A	0.9800
C14	H14A	0.9800	C15	C16	1.506(9)
C15	H15A	0.9700	C15	H15B	0.9700
C16	H16A	0.9600	C16	H16B	0.9600
C16	H16C	0.9600	C17	C18	1.526(8)
C17	H17A	0.9700	C17	H17B	0.9700
C18	H18A	0.9600	C18	H18B	0.9600
C18	H18C	0.9600	C19	C24	1.371(9)
C19	C20	1.408(9)	C20	C21	1.361(9)
C20	H20A	0.9300	C21	C22	1.380(9)
C21	H21A	0.9300	C22	C23	1.369(9)
C22	H22A	0.9300	C23	C24	1.390(10)
C23	H23A	0.9300	C24	H24A	0.9300
C25	C30	1.388(9)	C25	C26	1.388(9)
C25	H25A	0.9300	C26	C27	1.378(9)
C27	C28	1.381(9)	C27	H27A	0.9300
C28	C29	1.376(9)	C28	H28A	0.9300
C29	C30	1.355(9)	C29	H29A	0.9300
C30	H30A	0.9300	C31	C32	1.381(8)
C31	C36	1.403(9)	C32	C33	1.394(9)
C32	H32A	0.9300	C33	C34	1.350(10)

C33	H33A	0.9300	C34	C35	1.379(9)
C34	H34A	0.9300	C35	C36	1.384(9)
C35	H35A	0.9300	C36	H36A	0.9300
Zr2	C101	2.234(7)	Zr2	C104	2.264(7)
Zr2	C105	2.477(7)	Zr2	C112	2.503(8)
Zr2	C110	2.505(7)	Zr2	C114	2.507(8)
Zr2	C106	2.508(7)	Zr2	C109	2.514(7)
Zr2	C113	2.514(7)	Zr2	C111	2.518(7)
Zr2	C108	2.519(8)	Zr2	C107	2.523(8)
P2	C104	1.812(7)	P2	C125	1.830(7)
P2	C131	1.839(7)	C101	C102	1.337(9)
C101	C115	1.518(10)	C102	C103	1.499(9)
C102	C117	1.516(9)	C103	C104	1.367(9)
C103	C119	1.509(9)	C105	C109	1.404(9)
C105	C106	1.413(10)	C105	H10B	0.9800
C106	C107	1.378(10)	C106	H10C	0.9800
C107	C108	1.390(10)	C107	H10D	0.9800
C108	C109	1.407(10)	C108	H10E	0.9800
C109	H10F	0.9800	C110	C111	1.385(10)
C110	C114	1.391(10)	C110	H11B	0.9800
C111	C112	1.376(10)	C111	H11C	0.9800
C112	C113	1.410(10)	C112	H11D	0.9800
C113	C114	1.390(10)	C113	H11E	0.9800
C115	C116	1.474(10)	C115	H11F	0.9700
C115	H11G	0.9700	C116	H11H	0.9600
C116	H11I	0.9600	C116	H11J	0.9600
C117	C118	1.519(9)	C117	H11K	0.9700
C117	H11L	0.9700	C118	H11M	0.9600
C118	H11N	0.9600	C118	H11O	0.9600
C119	C120	1.368(9)	C119	C124	1.399(9)
C120	C121	1.381(9)	C120	H12B	0.9300
C121	C122	1.372(9)	C121	H12C	0.9300
C122	C123	1.353(9)	C122	H12D	0.9300
C123	C124	1.370(9)	C123	H12E	0.9300
C124	H12F	0.9300	C125	C130	1.375(9)
C125	C126	1.390(9)	C126	C127	1.366(10)
C126	H12G	0.9300	C127	C128	1.376(11)
C127	H12H	0.9300	C128	C129	1.382(10)
C128	H12I	0.9300	C129	C130	1.398(9)
C129	H12J	0.9300	C130	H13B	0.9300
C131	C132	1.374(9)	C131	C136	1.398(9)
C132	C133	1.388(10)	C132	H13C	0.9300
C133	C134	1.367(10)	C133	H13D	0.9300
C134	C135	1.395(10)	C134	H13E	0.9300
C135	C136	1.369(9)	C135	H13F	0.9300
C136	H13G	0.9300	C114	H11P	0.9800

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	Zr1	C4	79.4(3)	C1	Zr1	C5	131.5(2)
C4	Zr1	C5	108.5(3)	C1	Zr1	C9	106.5(3)
C4	Zr1	C9	84.5(3)	C5	Zr1	C9	32.6(2)
C1	Zr1	C13	131.2(2)	C4	Zr1	C13	100.3(3)
C5	Zr1	C13	95.4(3)	C9	Zr1	C13	122.1(3)
C1	Zr1	C12	103.2(3)	C4	Zr1	C12	78.7(2)
C5	Zr1	C12	125.3(3)	C9	Zr1	C12	142.3(3)
C13	Zr1	C12	32.5(2)	C1	Zr1	C11	77.2(2)
C4	Zr1	C11	92.4(2)	C5	Zr1	C11	146.3(3)
C9	Zr1	C11	174.6(3)	C13	Zr1	C11	54.0(2)
C12	Zr1	C11	32.3(2)	C1	Zr1	C10	86.0(3)
C4	Zr1	C10	124.9(3)	C5	Zr1	C10	120.4(3)
C9	Zr1	C10	150.1(3)	C13	Zr1	C10	53.9(2)
C12	Zr1	C10	53.5(3)	C11	Zr1	C10	32.5(2)
C1	Zr1	C14	117.9(3)	C4	Zr1	C14	130.9(2)
C5	Zr1	C14	93.3(3)	C9	Zr1	C14	125.9(3)
C13	Zr1	C14	32.5(2)	C12	Zr1	C14	53.3(3)
C11	Zr1	C14	53.5(3)	C10	Zr1	C14	32.2(2)
C1	Zr1	C8	78.4(3)	C4	Zr1	C8	95.2(3)
C5	Zr1	C8	53.6(3)	C9	Zr1	C8	32.5(2)
C13	Zr1	C8	148.5(3)	C12	Zr1	C8	173.2(3)
C11	Zr1	C8	152.6(3)	C10	Zr1	C8	133.3(3)
C14	Zr1	C8	131.9(3)	C1	Zr1	C6	114.2(3)
C4	Zr1	C6	137.6(3)	C5	Zr1	C6	31.9(2)
C9	Zr1	C6	53.4(3)	C13	Zr1	C6	98.7(3)
C12	Zr1	C6	130.5(3)	C11	Zr1	C6	129.1(3)
C10	Zr1	C6	96.8(3)	C14	Zr1	C6	80.1(3)
C8	Zr1	C6	53.0(3)	C1	Zr1	C7	83.6(3)
C4	Zr1	C7	127.0(3)	C5	Zr1	C7	52.7(3)
C9	Zr1	C7	53.2(3)	C13	Zr1	C7	127.6(3)
C12	Zr1	C7	154.3(3)	C11	Zr1	C7	131.8(3)
C10	Zr1	C7	103.2(3)	C14	Zr1	C7	101.5(3)
C8	Zr1	C7	31.9(2)	C6	Zr1	C7	31.6(2)
C4	P1	C31	104.4(3)	C4	P1	C26	101.9(3)
C31	P1	C26	100.8(3)	C2	C1	C15	121.6(7)
C2	C1	Zr1	110.7(5)	C15	C1	Zr1	127.6(6)
C1	C2	C3	120.3(6)	C1	C2	C17	123.7(7)
C3	C2	C17	115.8(7)	C4	C3	C19	123.6(6)
C4	C3	C2	119.9(6)	C19	C3	C2	116.4(6)
C3	C4	P1	118.1(5)	C3	C4	Zr1	107.9(5)
P1	C4	Zr1	132.4(4)	C6	C5	C9	108.5(7)

C6	C5	Zr1	75.4(4)	C9	C5	Zr1	73.9(4)
C6	C5	H5A	125.3	C9	C5	H5A	125.3
Zr1	C5	H5A	125.3	C7	C6	C5	108.2(8)
C7	C6	Zr1	74.5(4)	C5	C6	Zr1	72.7(4)
C7	C6	H6A	125.6	C5	C6	H6A	125.6
Zr1	C6	H6A	125.6	C6	C7	C8	109.0(8)
C6	C7	Zr1	73.9(4)	C8	C7	Zr1	73.6(4)
C6	C7	H7A	125.2	C8	C7	H7A	125.2
Zr1	C7	H7A	125.2	C7	C8	C9	107.2(7)
C7	C8	Zr1	74.5(4)	C9	C8	Zr1	72.7(4)
C7	C8	H8A	126.0	C9	C8	H8A	126.0
Zr1	C8	H8A	126.0	C5	C9	C8	107.1(8)
C5	C9	Zr1	73.5(4)	C8	C9	Zr1	74.7(4)
C5	C9	H9A	126.0	C8	C9	H9A	126.0
Zr1	C9	H9A	126.0	C14	C10	C11	107.9(7)
C14	C10	Zr1	74.3(4)	C11	C10	Zr1	73.7(4)
C14	C10	H10A	125.7	C11	C10	H10A	125.7
Zr1	C10	H10A	125.7	C12	C11	C10	107.5(7)
C12	C11	Zr1	73.6(4)	C10	C11	Zr1	73.8(4)
C12	C11	H11A	125.9	C10	C11	H11A	125.9
Zr1	C11	H11A	125.9	C11	C12	C13	108.9(7)
C11	C12	Zr1	74.1(4)	C13	C12	Zr1	73.6(4)
C11	C12	H12A	125.3	C13	C12	H12A	125.3
Zr1	C12	H12A	125.3	C12	C13	C14	107.1(7)
C12	C13	Zr1	73.9(4)	C14	C13	Zr1	74.6(4)
C12	C13	H13A	126.0	C14	C13	H13A	126.0
Zr1	C13	H13A	126.0	C10	C14	C13	108.5(7)
C10	C14	Zr1	73.5(4)	C13	C14	Zr1	72.9(4)
C10	C14	H14A	125.5	C13	C14	H14A	125.5
Zr1	C14	H14A	125.5	C16	C15	C1	113.9(6)
C16	C15	H15A	108.8	C1	C15	H15A	108.8
C16	C15	H15B	108.8	C1	C15	H15B	108.8
H15A	C15	H15B	107.7	C15	C16	H16A	109.5
C15	C16	H16B	109.5	H16A	C16	H16B	109.5
C15	C16	H16C	109.5	H16A	C16	H16C	109.5
H16B	C16	H16C	109.5	C2	C17	C18	112.2(5)
C2	C17	H17A	109.2	C18	C17	H17A	109.2
C2	C17	H17B	109.2	C18	C17	H17B	109.2
H17A	C17	H17B	107.9	C17	C18	H18A	109.5
C17	C18	H18B	109.5	H18A	C18	H18B	109.5
C17	C18	H18C	109.5	H18A	C18	H18C	109.5
H18B	C18	H18C	109.5	C24	C19	C20	116.5(7)
C24	C19	C3	125.2(6)	C20	C19	C3	118.3(7)
C21	C20	C19	121.6(7)	C21	C20	H20A	119.2
C19	C20	H20A	119.2	C20	C21	C22	120.2(7)
C20	C21	H21A	119.9	C22	C21	H21A	119.9

C23	C22	C21	120.1(7)	C23	C22	H22A	120.0
C21	C22	H22A	120.0	C22	C23	C24	119.0(7)
C22	C23	H23A	120.5	C24	C23	H23A	120.5
C19	C24	C23	122.6(7)	C19	C24	H24A	118.7
C23	C24	H24A	118.7	C30	C25	C26	120.1(7)
C30	C25	H25A	119.9	C26	C25	H25A	119.9
C27	C26	C25	118.0(6)	C27	C26	P1	119.7(5)
C25	C26	P1	122.1(6)	C26	C27	C28	121.8(7)
C26	C27	H27A	119.1	C28	C27	H27A	119.1
C29	C28	C27	119.0(7)	C29	C28	H28A	120.5
C27	C28	H28A	120.5	C30	C29	C28	120.3(7)
C30	C29	H29A	119.8	C28	C29	H29A	119.8
C29	C30	C25	120.7(7)	C29	C30	H30A	119.7
C25	C30	H30A	119.7	C32	C31	C36	116.3(7)
C32	C31	P1	117.5(6)	C36	C31	P1	126.2(5)
C31	C32	C33	122.0(7)	C31	C32	H32A	119.0
C33	C32	H32A	119.0	C34	C33	C32	120.2(7)
C34	C33	H33A	119.9	C32	C33	H33A	119.9
C33	C34	C35	120.0(7)	C33	C34	H34A	120.0
C35	C34	H34A	120.0	C34	C35	C36	119.8(7)
C34	C35	H35A	120.1	C36	C35	H35A	120.1
C35	C36	C31	121.6(7)	C35	C36	H36A	119.2
C31	C36	H36A	119.2	C101	Zr2	C104	81.7(3)
C101	Zr2	C105	130.9(3)	C104	Zr2	C105	108.4(3)
C101	Zr2	C112	101.1(3)	C104	Zr2	C112	78.6(3)
C105	Zr2	C112	127.9(3)	C101	Zr2	C110	94.2(3)
C104	Zr2	C110	130.0(3)	C105	Zr2	C110	111.3(3)
C112	Zr2	C110	53.1(3)	C101	Zr2	C114	126.5(3)
C104	Zr2	C114	126.0(3)	C105	Zr2	C114	87.0(3)
C112	Zr2	C114	53.5(3)	C110	Zr2	C114	32.2(2)
C101	Zr2	C106	111.1(3)	C104	Zr2	C106	137.8(2)
C105	Zr2	C106	32.9(2)	C112	Zr2	C106	133.0(3)
C110	Zr2	C106	90.2(3)	C114	Zr2	C106	79.6(3)
C101	Zr2	C109	107.2(3)	C104	Zr2	C109	84.0(3)
C105	Zr2	C109	32.7(2)	C112	Zr2	C109	144.1(3)
C110	Zr2	C109	142.8(3)	C114	Zr2	C109	119.2(3)
C106	Zr2	C109	54.0(3)	C101	Zr2	C113	132.2(3)
C104	Zr2	C113	94.0(3)	C105	Zr2	C113	95.8(3)
C112	Zr2	C113	32.6(2)	C110	Zr2	C113	53.2(3)
C114	Zr2	C113	32.2(2)	C106	Zr2	C113	103.7(3)
C109	Zr2	C113	119.7(3)	C101	Zr2	C111	80.3(3)
C104	Zr2	C111	99.2(3)	C105	Zr2	C111	140.1(3)
C112	Zr2	C111	31.8(2)	C110	Zr2	C111	32.0(2)
C114	Zr2	C111	53.2(3)	C106	Zr2	C111	122.1(3)
C109	Zr2	C111	172.2(3)	C113	Zr2	C111	53.3(3)
C101	Zr2	C108	78.1(3)	C104	Zr2	C108	93.6(3)

C105	Zr2	C108	53.9(3)	C112	Zr2	C108	172.2(3)
C110	Zr2	C108	134.6(3)	C114	Zr2	C108	133.1(3)
C106	Zr2	C108	53.5(3)	C109	Zr2	C108	32.5(2)
C113	Zr2	C108	149.6(3)	C111	Zr2	C108	153.0(3)
C101	Zr2	C107	81.0(3)	C104	Zr2	C107	125.3(3)
C105	Zr2	C107	53.5(3)	C112	Zr2	C107	155.8(3)
C110	Zr2	C107	102.8(3)	C114	Zr2	C107	105.7(3)
C106	Zr2	C107	31.8(2)	C109	Zr2	C107	53.3(3)
C113	Zr2	C107	134.3(3)	C111	Zr2	C107	128.0(3)
C108	Zr2	C107	32.0(2)	C104	P2	C125	101.7(3)
C104	P2	C131	105.5(3)	C125	P2	C131	99.2(3)
C102	C101	C115	119.4(7)	C102	C101	Zr2	108.5(5)
C115	C101	Zr2	131.0(5)	C101	C102	C103	120.4(6)
C101	C102	C117	122.4(7)	C103	C102	C117	117.0(7)
C104	C103	C102	123.5(7)	C104	C103	C119	120.3(7)
C102	C103	C119	116.2(6)	C103	C104	P2	117.4(5)
C103	C104	Zr2	104.8(5)	P2	C104	Zr2	136.7(4)
C109	C105	C106	108.0(7)	C109	C105	Zr2	75.1(4)
C106	C105	Zr2	74.7(4)	C109	C105	H10B	125.5
C106	C105	H10B	125.5	Zr2	C105	H10B	125.5
C107	C106	C105	107.4(8)	C107	C106	Zr2	74.7(4)
C105	C106	Zr2	72.3(4)	C107	C106	H10C	126.0
C105	C106	H10C	126.0	Zr2	C106	H10C	126.0
C106	C107	C108	109.6(8)	C106	C107	Zr2	73.5(5)
C108	C107	Zr2	73.8(5)	C106	C107	H10D	125.0
C108	C107	H10D	125.0	Zr2	C107	H10D	125.0
C107	C108	C109	107.7(8)	C107	C108	Zr2	74.2(5)
C109	C108	Zr2	73.6(4)	C107	C108	H10E	125.8
C109	C108	H10E	125.8	Zr2	C108	H10E	125.8
C105	C109	C108	107.4(8)	C105	C109	Zr2	72.2(4)
C108	C109	Zr2	74.0(4)	C105	C109	H10F	126.0
C108	C109	H10F	126.0	Zr2	C109	H10F	126.0
C111	C110	C114	108.4(8)	C111	C110	Zr2	74.5(4)
C114	C110	Zr2	73.9(4)	C111	C110	H11B	125.4
C114	C110	H11B	125.4	Zr2	C110	H11B	125.4
C112	C111	C110	108.3(8)	C112	C111	Zr2	73.5(4)
C110	C111	Zr2	73.5(4)	C112	C111	H11C	125.6
C110	C111	H11C	125.6	Zr2	C111	H11C	125.6
C111	C112	C113	108.1(8)	C111	C112	Zr2	74.7(5)
C113	C112	Zr2	74.1(4)	C111	C112	H11D	125.5
C113	C112	H11D	125.5	Zr2	C112	H11D	125.5
C114	C113	C112	107.3(7)	C114	C113	Zr2	73.6(5)
C112	C113	Zr2	73.3(4)	C114	C113	H11E	126.0
C112	C113	H11E	126.0	Zr2	C113	H11E	126.0
C116	C115	C101	113.4(7)	C116	C115	H11F	108.9
C101	C115	H11F	108.9	C116	C115	H11G	108.9

C101	C115	H11G	108.9	H11F	C115	H11G	107.7
C115	C116	H11H	109.5	C115	C116	H11I	109.5
H11H	C116	H11I	109.5	C115	C116	H11J	109.5
H11H	C116	H11J	109.5	H11I	C116	H11J	109.5
C102	C117	C118	111.5(6)	C102	C117	H11K	109.3
C118	C117	H11K	109.3	C102	C117	H11L	109.3
C118	C117	H11L	109.3	H11K	C117	H11L	108.0
C117	C118	H11M	109.5	C117	C118	H11N	109.5
H11M	C118	H11N	109.5	C117	C118	H11O	109.5
H11M	C118	H11O	109.5	H11N	C118	H11O	109.5
C120	C119	C124	117.0(7)	C120	C119	C103	125.3(7)
C124	C119	C103	117.7(7)	C119	C120	C121	121.4(7)
C119	C120	H12B	119.3	C121	C120	H12B	119.3
C122	C121	C120	120.0(7)	C122	C121	H12C	120.0
C120	C121	H12C	120.0	C123	C122	C121	120.0(7)
C123	C122	H12D	120.0	C121	C122	H12D	120.0
C122	C123	C124	120.0(7)	C122	C123	H12E	120.0
C124	C123	H12E	120.0	C123	C124	C119	121.6(7)
C123	C124	H12F	119.2	C119	C124	H12F	119.2
C130	C125	C126	117.9(7)	C130	C125	P2	123.8(6)
C126	C125	P2	118.1(6)	C127	C126	C125	121.4(8)
C127	C126	H12G	119.3	C125	C126	H12G	119.3
C126	C127	C128	120.8(8)	C126	C127	H12H	119.6
C128	C127	H12H	119.6	C127	C128	C129	119.0(8)
C127	C128	H12I	120.5	C129	C128	H12I	120.5
C128	C129	C130	119.8(8)	C128	C129	H12J	120.1
C130	C129	H12J	120.1	C125	C130	C129	121.1(7)
C125	C130	H13B	119.5	C129	C130	H13B	119.5
C132	C131	C136	117.2(7)	C132	C131	P2	117.6(6)
C136	C131	P2	125.2(6)	C131	C132	C133	122.4(7)
C131	C132	H13C	118.8	C133	C132	H13C	118.8
C134	C133	C132	119.5(8)	C134	C133	H13D	120.2
C132	C133	H13D	120.2	C133	C134	C135	119.3(7)
C133	C134	H13E	120.4	C135	C134	H13E	120.4
C136	C135	C134	120.5(8)	C136	C135	H13F	119.8
C134	C135	H13F	119.8	C135	C136	C131	121.1(7)
C135	C136	H13G	119.5	C131	C136	H13G	119.5
C113	C114	C110	107.9(8)	C113	C114	Zr2	74.2(5)
C110	C114	Zr2	73.8(4)	C113	C114	H11P	125.6
C110	C114	H11P	125.6	Zr2	C114	H11P	125.6

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C4	Zr1	C1	C2	-3.2(5)	C5	Zr1	C1	C2	-108.6(6)
C9	Zr1	C1	C2	-84.2(5)	C13	Zr1	C1	C2	91.3(6)
C12	Zr1	C1	C2	72.4(5)	C11	Zr1	C1	C2	91.8(5)
C10	Zr1	C1	C2	123.5(5)	C14	Zr1	C1	C2	127.7(5)
C8	Zr1	C1	C2	-100.8(5)	C6	Zr1	C1	C2	-140.9(5)
C7	Zr1	C1	C2	-132.7(5)	C4	Zr1	C1	C15	172.6(6)
C5	Zr1	C1	C15	67.2(7)	C9	Zr1	C1	C15	91.7(6)
C13	Zr1	C1	C15	-92.9(6)	C12	Zr1	C1	C15	-111.8(6)
C11	Zr1	C1	C15	-92.4(6)	C10	Zr1	C1	C15	-60.7(6)
C14	Zr1	C1	C15	-56.5(6)	C8	Zr1	C1	C15	75.1(6)
C6	Zr1	C1	C15	35.0(6)	C7	Zr1	C1	C15	43.1(6)
C15	C1	C2	C3	-179.7(5)	Zr1	C1	C2	C3	-3.6(8)
C15	C1	C2	C17	-4.4(10)	Zr1	C1	C2	C17	171.7(5)
C1	C2	C3	C4	13.6(9)	C17	C2	C3	C4	-162.0(6)
C1	C2	C3	C19	-163.9(6)	C17	C2	C3	C19	20.5(8)
C19	C3	C4	P1	-5.2(8)	C2	C3	C4	P1	177.4(4)
C19	C3	C4	Zr1	162.5(5)	C2	C3	C4	Zr1	-14.8(7)
C31	P1	C4	C3	154.5(5)	C26	P1	C4	C3	-100.9(5)
C31	P1	C4	Zr1	-9.6(5)	C26	P1	C4	Zr1	95.0(4)
C1	Zr1	C4	C3	9.5(4)	C5	Zr1	C4	C3	140.0(4)
C9	Zr1	C4	C3	117.5(5)	C13	Zr1	C4	C3	-120.8(4)
C12	Zr1	C4	C3	-96.4(4)	C11	Zr1	C4	C3	-67.0(4)
C10	Zr1	C4	C3	-67.9(5)	C14	Zr1	C4	C3	-108.3(5)
C8	Zr1	C4	C3	86.7(5)	C6	Zr1	C4	C3	123.9(5)
C7	Zr1	C4	C3	83.2(5)	C1	Zr1	C4	P1	174.9(4)
C5	Zr1	C4	P1	-54.7(5)	C9	Zr1	C4	P1	-77.2(5)
C13	Zr1	C4	P1	44.5(4)	C12	Zr1	C4	P1	69.0(4)
C11	Zr1	C4	P1	98.4(4)	C10	Zr1	C4	P1	97.5(5)
C14	Zr1	C4	P1	57.0(6)	C8	Zr1	C4	P1	-108.0(4)
C6	Zr1	C4	P1	-70.8(5)	C7	Zr1	C4	P1	-111.5(4)
C1	Zr1	C5	C6	-67.3(7)	C4	Zr1	C5	C6	-159.4(5)
C9	Zr1	C5	C6	-114.6(7)	C13	Zr1	C5	C6	97.9(5)
C12	Zr1	C5	C6	111.6(5)	C11	Zr1	C5	C6	75.1(7)
C10	Zr1	C5	C6	47.0(6)	C14	Zr1	C5	C6	65.3(5)
C8	Zr1	C5	C6	-76.8(5)	C7	Zr1	C5	C6	-36.5(5)
C1	Zr1	C5	C9	47.3(7)	C4	Zr1	C5	C9	-44.8(6)
C13	Zr1	C5	C9	-147.6(6)	C12	Zr1	C5	C9	-133.9(5)
C11	Zr1	C5	C9	-170.3(5)	C10	Zr1	C5	C9	161.5(5)
C14	Zr1	C5	C9	179.9(6)	C8	Zr1	C5	C9	37.8(5)
C6	Zr1	C5	C9	114.6(7)	C7	Zr1	C5	C9	78.0(5)

C9	C5	C6	C7	-0.4(9)	Zr1	C5	C6	C7	66.7(5)
C9	C5	C6	Zr1	-67.1(5)	C1	Zr1	C6	C7	15.6(7)
C4	Zr1	C6	C7	-85.5(7)	C5	Zr1	C6	C7	-115.2(7)
C9	Zr1	C6	C7	-77.5(5)	C13	Zr1	C6	C7	158.7(6)
C12	Zr1	C6	C7	151.0(5)	C11	Zr1	C6	C7	108.6(6)
C10	Zr1	C6	C7	104.3(6)	C14	Zr1	C6	C7	131.9(6)
C8	Zr1	C6	C7	-36.5(5)	C1	Zr1	C6	C5	130.8(5)
C4	Zr1	C6	C5	29.7(7)	C9	Zr1	C6	C5	37.7(4)
C13	Zr1	C6	C5	-86.2(5)	C12	Zr1	C6	C5	-93.8(6)
C11	Zr1	C6	C5	-136.2(5)	C10	Zr1	C6	C5	-140.6(5)
C14	Zr1	C6	C5	-112.9(6)	C8	Zr1	C6	C5	78.6(5)
C7	Zr1	C6	C5	115.2(7)	C5	C6	C7	C8	0.3(9)
Zr1	C6	C7	C8	65.8(5)	C5	C6	C7	Zr1	-65.4(5)
C1	Zr1	C7	C6	-165.7(6)	C4	Zr1	C7	C6	122.7(6)
C5	Zr1	C7	C6	37.0(5)	C9	Zr1	C7	C6	78.2(5)
C13	Zr1	C7	C6	-27.0(7)	C12	Zr1	C7	C6	-58.3(9)
C11	Zr1	C7	C6	-99.2(6)	C10	Zr1	C7	C6	-81.4(6)
C14	Zr1	C7	C6	-48.4(6)	C8	Zr1	C7	C6	116.0(7)
C1	Zr1	C7	C8	78.3(6)	C4	Zr1	C7	C8	6.7(6)
C5	Zr1	C7	C8	-79.1(5)	C9	Zr1	C7	C8	-37.8(5)
C13	Zr1	C7	C8	-143.0(5)	C12	Zr1	C7	C8	-174.4(6)
C11	Zr1	C7	C8	144.8(5)	C10	Zr1	C7	C8	162.6(5)
C14	Zr1	C7	C8	-164.4(5)	C6	Zr1	C7	C8	-116.0(7)
C6	C7	C8	C9	-0.1(8)	Zr1	C7	C8	C9	65.9(5)
C6	C7	C8	Zr1	-66.0(5)	C1	Zr1	C8	C7	-96.6(6)
C4	Zr1	C8	C7	-174.6(5)	C5	Zr1	C8	C7	76.2(5)
C9	Zr1	C8	C7	114.1(7)	C13	Zr1	C8	C7	65.9(9)
C12	Zr1	C8	C7	159(2)	C11	Zr1	C8	C7	-69.1(8)
C10	Zr1	C8	C7	-23.5(7)	C14	Zr1	C8	C7	20.7(7)
C6	Zr1	C8	C7	36.1(4)	C1	Zr1	C8	C9	149.3(6)
C4	Zr1	C8	C9	71.3(6)	C5	Zr1	C8	C9	-37.9(5)
C13	Zr1	C8	C9	-48.2(9)	C12	Zr1	C8	C9	45(2)
C11	Zr1	C8	C9	176.8(6)	C10	Zr1	C8	C9	-137.6(6)
C14	Zr1	C8	C9	-93.4(7)	C6	Zr1	C8	C9	-78.0(5)
C7	Zr1	C8	C9	-114.1(7)	C6	C5	C9	C8	0.4(8)
Zr1	C5	C9	C8	-67.7(5)	C6	C5	C9	Zr1	68.1(5)
C7	C8	C9	C5	-0.2(8)	Zr1	C8	C9	C5	66.9(5)
C7	C8	C9	Zr1	-67.0(5)	C1	Zr1	C9	C5	-145.0(6)
C4	Zr1	C9	C5	137.8(6)	C13	Zr1	C9	C5	39.1(6)
C12	Zr1	C9	C5	74.4(7)	C11	Zr1	C9	C5	82(3)
C10	Zr1	C9	C5	-33.3(9)	C14	Zr1	C9	C5	-0.1(7)
C8	Zr1	C9	C5	-113.5(7)	C6	Zr1	C9	C5	-36.8(5)
C7	Zr1	C9	C5	-76.4(5)	C1	Zr1	C9	C8	-31.4(6)
C4	Zr1	C9	C8	-108.6(6)	C5	Zr1	C9	C8	113.5(7)
C13	Zr1	C9	C8	152.6(5)	C12	Zr1	C9	C8	-172.1(5)
C11	Zr1	C9	C8	-164(3)	C10	Zr1	C9	C8	80.3(9)

C14	Zr1	C9	C8	113.5(6)	C6	Zr1	C9	C8	76.8(5)
C7	Zr1	C9	C8	37.1(4)	C1	Zr1	C10	C14	173.1(5)
C4	Zr1	C10	C14	-112.9(5)	C5	Zr1	C10	C14	36.3(6)
C9	Zr1	C10	C14	56.3(8)	C13	Zr1	C10	C14	-36.7(4)
C12	Zr1	C10	C14	-77.3(5)	C11	Zr1	C10	C14	-114.5(7)
C8	Zr1	C10	C14	103.1(5)	C6	Zr1	C10	C14	59.2(5)
C7	Zr1	C10	C14	90.6(5)	C1	Zr1	C10	C11	-72.4(5)
C4	Zr1	C10	C11	1.7(6)	C5	Zr1	C10	C11	150.8(5)
C9	Zr1	C10	C11	170.9(6)	C13	Zr1	C10	C11	77.9(5)
C12	Zr1	C10	C11	37.2(4)	C14	Zr1	C10	C11	114.5(7)
C8	Zr1	C10	C11	-142.4(5)	C6	Zr1	C10	C11	173.7(5)
C7	Zr1	C10	C11	-154.9(5)	C14	C10	C11	C12	0.5(8)
Zr1	C10	C11	C12	-66.5(5)	C14	C10	C11	Zr1	67.0(5)
C1	Zr1	C11	C12	-142.9(5)	C4	Zr1	C11	C12	-64.3(5)
C5	Zr1	C11	C12	65.1(8)	C9	Zr1	C11	C12	-9(3)
C13	Zr1	C11	C12	36.7(4)	C10	Zr1	C11	C12	114.3(7)
C14	Zr1	C11	C12	77.3(5)	C8	Zr1	C11	C12	-170.4(6)
C6	Zr1	C11	C12	106.2(6)	C7	Zr1	C11	C12	148.0(5)
C1	Zr1	C11	C10	102.8(5)	C4	Zr1	C11	C10	-178.6(5)
C5	Zr1	C11	C10	-49.3(8)	C9	Zr1	C11	C10	-123(3)
C13	Zr1	C11	C10	-77.6(5)	C12	Zr1	C11	C10	-114.3(7)
C14	Zr1	C11	C10	-37.1(4)	C8	Zr1	C11	C10	75.2(8)
C6	Zr1	C11	C10	-8.1(6)	C7	Zr1	C11	C10	33.7(6)
C10	C11	C12	C13	0.7(8)	Zr1	C11	C12	C13	-65.9(5)
C10	C11	C12	Zr1	66.6(5)	C1	Zr1	C12	C11	37.2(5)
C4	Zr1	C12	C11	113.3(5)	C5	Zr1	C12	C11	-141.9(5)
C9	Zr1	C12	C11	178.6(5)	C13	Zr1	C12	C11	-115.8(7)
C10	Zr1	C12	C11	-37.6(4)	C14	Zr1	C12	C11	-77.9(5)
C8	Zr1	C12	C11	140(2)	C6	Zr1	C12	C11	-101.6(6)
C7	Zr1	C12	C11	-65.8(8)	C1	Zr1	C12	C13	153.0(5)
C4	Zr1	C12	C13	-130.8(5)	C5	Zr1	C12	C13	-26.0(6)
C9	Zr1	C12	C13	-65.6(7)	C11	Zr1	C12	C13	115.8(7)
C10	Zr1	C12	C13	78.3(5)	C14	Zr1	C12	C13	37.9(4)
C8	Zr1	C12	C13	-104(2)	C6	Zr1	C12	C13	14.2(7)
C7	Zr1	C12	C13	50.1(8)	C11	C12	C13	C14	-1.6(8)
Zr1	C12	C13	C14	-67.8(5)	C11	C12	C13	Zr1	66.2(5)
C1	Zr1	C13	C12	-35.9(6)	C4	Zr1	C13	C12	49.0(5)
C5	Zr1	C13	C12	158.9(5)	C9	Zr1	C13	C12	138.9(5)
C11	Zr1	C13	C12	-36.5(4)	C10	Zr1	C13	C12	-77.0(5)
C14	Zr1	C13	C12	-113.4(7)	C8	Zr1	C13	C12	167.2(6)
C6	Zr1	C13	C12	-169.1(5)	C7	Zr1	C13	C12	-155.2(5)
C1	Zr1	C13	C14	77.4(6)	C4	Zr1	C13	C14	162.3(5)
C5	Zr1	C13	C14	-87.7(6)	C9	Zr1	C13	C14	-107.7(5)
C12	Zr1	C13	C14	113.4(7)	C11	Zr1	C13	C14	76.9(5)
C10	Zr1	C13	C14	36.3(4)	C8	Zr1	C13	C14	-79.4(8)
C6	Zr1	C13	C14	-55.8(6)	C7	Zr1	C13	C14	-41.9(6)

C11	C10	C14	C13	-1.5(8)	Zr1	C10	C14	C13	65.0(5)
C11	C10	C14	Zr1	-66.6(5)	C12	C13	C14	C10	2.0(8)
Zr1	C13	C14	C10	-65.4(5)	C12	C13	C14	Zr1	67.4(5)
C1	Zr1	C14	C10	-7.8(6)	C4	Zr1	C14	C10	92.7(6)
C5	Zr1	C14	C10	-149.3(5)	C9	Zr1	C14	C10	-149.2(5)
C13	Zr1	C14	C10	116.0(7)	C12	Zr1	C14	C10	78.0(5)
C11	Zr1	C14	C10	37.5(4)	C8	Zr1	C14	C10	-107.7(6)
C6	Zr1	C14	C10	-120.1(5)	C7	Zr1	C14	C10	-96.7(5)
C1	Zr1	C14	C13	-123.8(5)	C4	Zr1	C14	C13	-23.3(7)
C5	Zr1	C14	C13	94.8(5)	C9	Zr1	C14	C13	94.8(6)
C12	Zr1	C14	C13	-37.9(4)	C11	Zr1	C14	C13	-78.5(5)
C10	Zr1	C14	C13	-116.0(7)	C8	Zr1	C14	C13	136.4(5)
C6	Zr1	C14	C13	124.0(6)	C7	Zr1	C14	C13	147.4(5)
C2	C1	C15	C16	-82.3(9)	Zr1	C1	C15	C16	102.2(7)
C1	C2	C17	C18	-100.3(8)	C3	C2	C17	C18	75.2(7)
C4	C3	C19	C24	69.0(9)	C2	C3	C19	C24	-113.5(7)
C4	C3	C19	C20	-110.1(7)	C2	C3	C19	C20	67.3(8)
C24	C19	C20	C21	-0.4(10)	C3	C19	C20	C21	178.8(6)
C19	C20	C21	C22	0.6(10)	C20	C21	C22	C23	-0.9(11)
C21	C22	C23	C24	1.1(11)	C20	C19	C24	C23	0.6(10)
C3	C19	C24	C23	-178.5(6)	C22	C23	C24	C19	-1.0(11)
C30	C25	C26	C27	-0.9(10)	C30	C25	C26	P1	174.7(6)
C4	P1	C26	C27	-155.4(6)	C31	P1	C26	C27	-48.0(6)
C4	P1	C26	C25	29.1(6)	C31	P1	C26	C25	136.5(6)
C25	C26	C27	C28	-0.4(10)	P1	C26	C27	C28	-176.1(5)
C26	C27	C28	C29	1.4(11)	C27	C28	C29	C30	-1.0(11)
C28	C29	C30	C25	-0.3(11)	C26	C25	C30	C29	1.3(11)
C4	P1	C31	C32	-104.1(6)	C26	P1	C31	C32	150.5(6)
C4	P1	C31	C36	76.3(7)	C26	P1	C31	C36	-29.1(7)
C36	C31	C32	C33	-1.2(10)	P1	C31	C32	C33	179.1(6)
C31	C32	C33	C34	2.6(11)	C32	C33	C34	C35	-1.8(12)
C33	C34	C35	C36	-0.3(12)	C34	C35	C36	C31	1.7(12)
C32	C31	C36	C35	-0.9(11)	P1	C31	C36	C35	178.7(6)
C104	Zr2	C101	C102	-0.2(5)	C105	Zr2	C101	C102	-107.4(6)
C112	Zr2	C101	C102	76.4(5)	C110	Zr2	C101	C102	129.6(5)
C114	Zr2	C101	C102	128.9(5)	C106	Zr2	C101	C102	-138.5(5)
C109	Zr2	C101	C102	-81.2(5)	C113	Zr2	C101	C102	87.6(6)
C111	Zr2	C101	C102	100.6(6)	C108	Zr2	C101	C102	-95.7(6)
C107	Zr2	C101	C102	-128.1(6)	C104	Zr2	C101	C115	167.4(7)
C105	Zr2	C101	C115	60.2(8)	C112	Zr2	C101	C115	-116.0(7)
C110	Zr2	C101	C115	-62.8(7)	C114	Zr2	C101	C115	-63.5(8)
C106	Zr2	C101	C115	29.1(7)	C109	Zr2	C101	C115	86.3(7)
C113	Zr2	C101	C115	-104.8(7)	C111	Zr2	C101	C115	-91.8(7)
C108	Zr2	C101	C115	71.9(7)	C107	Zr2	C101	C115	39.4(7)
C115	C101	C102	C103	-175.1(6)	Zr2	C101	C102	C103	-5.8(8)
C115	C101	C102	C117	-1.6(11)	Zr2	C101	C102	C117	167.7(5)

C101	C102	C103	C104	13.4(10)	C117	C102	C103	C104	-160.5(7)
C101	C102	C103	C119	-164.4(7)	C117	C102	C103	C119	21.7(9)
C102	C103	C104	P2	178.6(5)	C119	C103	C104	P2	-3.7(9)
C102	C103	C104	Zr2	-11.7(8)	C119	C103	C104	Zr2	165.9(5)
C125	P2	C104	C103	-94.7(6)	C131	P2	C104	C103	162.1(5)
C125	P2	C104	Zr2	99.9(5)	C131	P2	C104	Zr2	-3.2(6)
C101	Zr2	C104	C103	6.1(5)	C105	Zr2	C104	C103	136.5(5)
C112	Zr2	C104	C103	-97.1(5)	C110	Zr2	C104	C103	-82.5(6)
C114	Zr2	C104	C103	-123.4(5)	C106	Zr2	C104	C103	118.5(5)
C109	Zr2	C104	C103	114.5(5)	C113	Zr2	C104	C103	-126.1(5)
C111	Zr2	C104	C103	-72.7(5)	C108	Zr2	C104	C103	83.5(5)
C107	Zr2	C104	C103	78.8(5)	C101	Zr2	C104	P2	172.6(5)
C105	Zr2	C104	P2	-56.9(5)	C112	Zr2	C104	P2	69.4(5)
C110	Zr2	C104	P2	84.1(6)	C114	Zr2	C104	P2	43.1(6)
C106	Zr2	C104	P2	-75.0(6)	C109	Zr2	C104	P2	-79.0(5)
C113	Zr2	C104	P2	40.5(5)	C111	Zr2	C104	P2	93.9(5)
C108	Zr2	C104	P2	-110.0(5)	C107	Zr2	C104	P2	-114.7(5)
C101	Zr2	C105	C109	51.2(6)	C104	Zr2	C105	C109	-43.7(5)
C112	Zr2	C105	C109	-133.5(5)	C110	Zr2	C105	C109	167.5(5)
C114	Zr2	C105	C109	-170.8(5)	C106	Zr2	C105	C109	113.8(7)
C113	Zr2	C105	C109	-139.8(5)	C111	Zr2	C105	C109	-175.0(5)
C108	Zr2	C105	C109	37.1(5)	C107	Zr2	C105	C109	77.1(5)
C101	Zr2	C105	C106	-62.5(6)	C104	Zr2	C105	C106	-157.5(5)
C112	Zr2	C105	C106	112.8(5)	C110	Zr2	C105	C106	53.7(6)
C114	Zr2	C105	C106	75.4(5)	C109	Zr2	C105	C106	-113.8(7)
C113	Zr2	C105	C106	106.4(5)	C111	Zr2	C105	C106	71.2(7)
C108	Zr2	C105	C106	-76.7(5)	C107	Zr2	C105	C106	-36.7(5)
C109	C105	C106	C107	-1.3(8)	Zr2	C105	C106	C107	67.1(5)
C109	C105	C106	Zr2	-68.4(5)	C101	Zr2	C106	C107	19.7(6)
C104	Zr2	C106	C107	-81.5(7)	C105	Zr2	C106	C107	-114.3(7)
C112	Zr2	C106	C107	149.6(6)	C110	Zr2	C106	C107	114.4(6)
C114	Zr2	C106	C107	145.0(6)	C109	Zr2	C106	C107	-76.7(5)
C113	Zr2	C106	C107	166.4(5)	C111	Zr2	C106	C107	111.5(6)
C108	Zr2	C106	C107	-36.1(5)	C101	Zr2	C106	C105	134.0(5)
C104	Zr2	C106	C105	32.8(7)	C112	Zr2	C106	C105	-96.1(6)
C110	Zr2	C106	C105	-131.3(5)	C114	Zr2	C106	C105	-100.7(6)
C109	Zr2	C106	C105	37.6(4)	C113	Zr2	C106	C105	-79.3(5)
C111	Zr2	C106	C105	-134.2(5)	C108	Zr2	C106	C105	78.2(5)
C107	Zr2	C106	C105	114.3(7)	C105	C106	C107	C108	0.1(9)
Zr2	C106	C107	C108	65.6(6)	C105	C106	C107	Zr2	-65.5(5)
C101	Zr2	C107	C106	-161.4(6)	C104	Zr2	C107	C106	125.6(5)
C105	Zr2	C107	C106	38.1(5)	C112	Zr2	C107	C106	-64.4(9)
C110	Zr2	C107	C106	-69.1(6)	C114	Zr2	C107	C106	-35.9(6)
C109	Zr2	C107	C106	79.1(5)	C113	Zr2	C107	C106	-18.6(7)
C111	Zr2	C107	C106	-91.2(6)	C108	Zr2	C107	C106	116.7(8)
C101	Zr2	C107	C108	81.9(5)	C104	Zr2	C107	C108	8.9(6)

C105	Zr2	C107	C108	-78.6(5)	C112	Zr2	C107	C108	178.9(7)
C110	Zr2	C107	C108	174.2(5)	C114	Zr2	C107	C108	-152.6(5)
C106	Zr2	C107	C108	-116.7(8)	C109	Zr2	C107	C108	-37.6(5)
C113	Zr2	C107	C108	-135.3(5)	C111	Zr2	C107	C108	152.1(5)
C106	C107	C108	C109	1.1(9)	Zr2	C107	C108	C109	66.5(5)
C106	C107	C108	Zr2	-65.4(6)	C101	Zr2	C108	C107	-92.1(6)
C104	Zr2	C108	C107	-172.8(5)	C105	Zr2	C108	C107	77.0(5)
C112	Zr2	C108	C107	-177(2)	C110	Zr2	C108	C107	-7.9(7)
C114	Zr2	C108	C107	37.3(7)	C106	Zr2	C108	C107	35.9(5)
C109	Zr2	C108	C107	114.4(7)	C113	Zr2	C108	C107	83.1(8)
C111	Zr2	C108	C107	-54.4(9)	C101	Zr2	C108	C109	153.6(6)
C104	Zr2	C108	C109	72.9(5)	C105	Zr2	C108	C109	-37.3(4)
C112	Zr2	C108	C109	69(2)	C110	Zr2	C108	C109	-122.3(6)
C114	Zr2	C108	C109	-77.1(7)	C106	Zr2	C108	C109	-78.5(5)
C113	Zr2	C108	C109	-31.3(9)	C111	Zr2	C108	C109	-168.8(6)
C107	Zr2	C108	C109	-114.4(7)	C106	C105	C109	C108	2.0(8)
Zr2	C105	C109	C108	-66.1(5)	C106	C105	C109	Zr2	68.1(5)
C107	C108	C109	C105	-1.9(8)	Zr2	C108	C109	C105	65.0(5)
C107	C108	C109	Zr2	-66.9(5)	C101	Zr2	C109	C105	-141.9(5)
C104	Zr2	C109	C105	138.8(5)	C112	Zr2	C109	C105	77.6(7)
C110	Zr2	C109	C105	-19.5(7)	C114	Zr2	C109	C105	10.5(6)
C106	Zr2	C109	C105	-38.0(4)	C113	Zr2	C109	C105	47.6(6)
C111	Zr2	C109	C105	24(3)	C108	Zr2	C109	C105	-114.8(7)
C107	Zr2	C109	C105	-77.7(5)	C101	Zr2	C109	C108	-27.1(6)
C104	Zr2	C109	C108	-106.5(6)	C105	Zr2	C109	C108	114.8(7)
C112	Zr2	C109	C108	-167.6(5)	C110	Zr2	C109	C108	95.3(7)
C114	Zr2	C109	C108	125.3(6)	C106	Zr2	C109	C108	76.8(5)
C113	Zr2	C109	C108	162.4(5)	C111	Zr2	C109	C108	139(2)
C107	Zr2	C109	C108	37.0(5)	C101	Zr2	C110	C111	-64.1(6)
C104	Zr2	C110	C111	18.5(7)	C105	Zr2	C110	C111	158.7(5)
C112	Zr2	C110	C111	36.6(5)	C114	Zr2	C110	C111	114.8(8)
C106	Zr2	C110	C111	-175.3(6)	C109	Zr2	C110	C111	169.8(5)
C113	Zr2	C110	C111	77.7(6)	C108	Zr2	C110	C111	-141.6(5)
C107	Zr2	C110	C111	-145.9(6)	C101	Zr2	C110	C114	-179.0(6)
C104	Zr2	C110	C114	-96.3(6)	C105	Zr2	C110	C114	43.8(6)
C112	Zr2	C110	C114	-78.3(6)	C106	Zr2	C110	C114	69.8(6)
C109	Zr2	C110	C114	55.0(8)	C113	Zr2	C110	C114	-37.2(5)
C111	Zr2	C110	C114	-114.8(8)	C108	Zr2	C110	C114	103.6(6)
C107	Zr2	C110	C114	99.3(6)	C114	C110	C111	C112	0.9(9)
Zr2	C110	C111	C112	-65.8(6)	C114	C110	C111	Zr2	66.8(5)
C101	Zr2	C111	C112	-130.1(6)	C104	Zr2	C111	C112	-50.3(6)
C105	Zr2	C111	C112	83.5(7)	C110	Zr2	C111	C112	115.4(8)
C114	Zr2	C111	C112	78.2(5)	C106	Zr2	C111	C112	120.9(6)
C109	Zr2	C111	C112	63(3)	C113	Zr2	C111	C112	37.8(5)
C108	Zr2	C111	C112	-167.5(6)	C107	Zr2	C111	C112	159.4(5)
C101	Zr2	C111	C110	114.5(6)	C104	Zr2	C111	C110	-165.7(5)

C105	Zr2	C111	C110	-31.9(8)	C112	Zr2	C111	C110	-115.4(8)
C114	Zr2	C111	C110	-37.2(5)	C106	Zr2	C111	C110	5.5(7)
C109	Zr2	C111	C110	-52(3)	C113	Zr2	C111	C110	-77.6(5)
C108	Zr2	C111	C110	77.1(8)	C107	Zr2	C111	C110	44.0(7)
C110	C111	C112	C113	-1.3(9)	Zr2	C111	C112	C113	-67.1(5)
C110	C111	C112	Zr2	65.8(6)	C101	Zr2	C112	C111	50.2(6)
C104	Zr2	C112	C111	129.2(6)	C105	Zr2	C112	C111	-126.2(6)
C110	Zr2	C112	C111	-36.8(5)	C114	Zr2	C112	C111	-77.3(5)
C106	Zr2	C112	C111	-83.0(7)	C109	Zr2	C112	C111	-168.1(5)
C113	Zr2	C112	C111	-114.4(7)	C108	Zr2	C112	C111	133(2)
C107	Zr2	C112	C111	-42.5(10)	C101	Zr2	C112	C113	164.6(5)
C104	Zr2	C112	C113	-116.4(6)	C105	Zr2	C112	C113	-11.8(7)
C110	Zr2	C112	C113	77.6(5)	C114	Zr2	C112	C113	37.1(4)
C106	Zr2	C112	C113	31.4(7)	C109	Zr2	C112	C113	-53.7(7)
C111	Zr2	C112	C113	114.4(7)	C108	Zr2	C112	C113	-112(2)
C107	Zr2	C112	C113	71.8(10)	C111	C112	C113	C114	1.2(9)
Zr2	C112	C113	C114	-66.3(5)	C111	C112	C113	Zr2	67.5(6)
C101	Zr2	C113	C114	93.7(6)	C104	Zr2	C113	C114	176.0(5)
C105	Zr2	C113	C114	-75.0(5)	C112	Zr2	C113	C114	114.3(7)
C110	Zr2	C113	C114	37.3(5)	C106	Zr2	C113	C114	-42.6(6)
C109	Zr2	C113	C114	-98.7(5)	C111	Zr2	C113	C114	77.5(5)
C108	Zr2	C113	C114	-80.0(8)	C107	Zr2	C113	C114	-32.6(7)
C101	Zr2	C113	C112	-20.7(7)	C104	Zr2	C113	C112	61.7(6)
C105	Zr2	C113	C112	170.6(6)	C110	Zr2	C113	C112	-77.1(5)
C114	Zr2	C113	C112	-114.3(7)	C106	Zr2	C113	C112	-156.9(5)
C109	Zr2	C113	C112	147.0(5)	C111	Zr2	C113	C112	-36.8(5)
C108	Zr2	C113	C112	165.7(6)	C107	Zr2	C113	C112	-146.9(6)
C102	C101	C115	C116	-148.2(7)	Zr2	C101	C115	C116	45.4(10)
C101	C102	C117	C118	-83.5(9)	C103	C102	C117	C118	90.2(8)
C104	C103	C119	C120	95.3(9)	C102	C103	C119	C120	-86.9(8)
C104	C103	C119	C124	-87.3(8)	C102	C103	C119	C124	90.6(8)
C124	C119	C120	C121	-1.0(10)	C103	C119	C120	C121	176.5(7)
C119	C120	C121	C122	0.5(11)	C120	C121	C122	C123	0.6(11)
C121	C122	C123	C124	-1.0(11)	C122	C123	C124	C119	0.5(11)
C120	C119	C124	C123	0.5(10)	C103	C119	C124	C123	-177.2(7)
C104	P2	C125	C130	23.5(7)	C131	P2	C125	C130	131.5(6)
C104	P2	C125	C126	-161.7(6)	C131	P2	C125	C126	-53.7(6)
C130	C125	C126	C127	-0.2(11)	P2	C125	C126	C127	-175.3(6)
C125	C126	C127	C128	0.0(12)	C126	C127	C128	C129	0.3(12)
C127	C128	C129	C130	-0.4(11)	C126	C125	C130	C129	0.2(11)
P2	C125	C130	C129	175.0(5)	C128	C129	C130	C125	0.2(11)
C104	P2	C131	C132	-114.8(6)	C125	P2	C131	C132	140.3(6)
C104	P2	C131	C136	65.9(7)	C125	P2	C131	C136	-39.0(7)
C136	C131	C132	C133	-2.4(11)	P2	C131	C132	C133	178.3(6)
C131	C132	C133	C134	1.4(12)	C132	C133	C134	C135	0.9(12)
C133	C134	C135	C136	-2.1(12)	C134	C135	C136	C131	1.1(11)

C132	C131	C136	C135	1.1(11)	P2	C131	C136	C135	-179.6(6)
C112	C113	C114	C110	-0.6(9)	Zr2	C113	C114	C110	-66.7(5)
C112	C113	C114	Zr2	66.1(5)	C111	C110	C114	C113	-0.2(9)
Zr2	C110	C114	C113	67.0(6)	C111	C110	C114	Zr2	-67.1(5)
C101	Zr2	C114	C113	-113.3(6)	C104	Zr2	C114	C113	-4.9(7)
C105	Zr2	C114	C113	105.7(5)	C112	Zr2	C114	C113	-37.7(5)
C110	Zr2	C114	C113	-114.5(8)	C106	Zr2	C114	C113	138.1(6)
C109	Zr2	C114	C113	100.1(5)	C111	Zr2	C114	C113	-77.6(5)
C108	Zr2	C114	C113	136.9(5)	C107	Zr2	C114	C113	156.4(5)
C101	Zr2	C114	C110	1.3(7)	C104	Zr2	C114	C110	109.6(6)
C105	Zr2	C114	C110	-139.7(6)	C112	Zr2	C114	C110	76.9(6)
C106	Zr2	C114	C110	-107.4(6)	C109	Zr2	C114	C110	-145.4(6)
C113	Zr2	C114	C110	114.5(8)	C111	Zr2	C114	C110	36.9(5)
C108	Zr2	C114	C110	-108.5(6)	C107	Zr2	C114	C110	-89.1(6)

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(1) XS: Program for the Solution of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(2) XL: Program for the Refinement of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(3) Least-Squares:

Function minimized $\Sigma w\,(|Fo|^2 - |Fc|^2)^2$

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|Fo|^2 - |Fc|^2)^2/(N_o - N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

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(9) XP: Molecular Graphics program. Part of the SHELXTL Structure Determination Package. Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

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(12)XPREP:(v 5.03) Part of the SHELXTL Crystal Structure Determination Package,
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