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Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A^2)
H(7021)	0.431	0.353	0.753	12.2
H(7031)	0.233	0.427	0.688	13.6
H(7041)	0.059	0.456	0.758	10.4
H(7051)	0.087	0.419	0.884	8.4
H(7061)	0.278	0.351	0.945	8.9

Hydrogens included in calculation of structure factors but not refined
B(H)=1.3*B(C)

Table of General Temperature Factor Expressions - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
Ti	2.41(4)	2.58(4)	2.49(4)	0.00(3)	0.89(3)	0.06(3)	2.46(2)
O(5)	2.8(1)	3.0(2)	3.0(1)	0.3(1)	1.3(1)	0.4(1)	2.81(8)
O(6)	2.8(2)	2.8(2)	2.8(2)	-0.1(1)	0.5(1)	0.2(1)	2.84(8)
N(1)	2.8(2)	3.1(2)	3.0(2)	0.3(2)	0.9(2)	0.0(2)	3.0(1)
N(4)	2.5(2)	3.0(2)	2.9(2)	-0.1(2)	0.9(1)	-0.2(2)	2.8(1)
C(2)	2.9(2)	2.8(2)	3.0(2)	-0.4(2)	1.2(2)	0.2(2)	2.9(1)
C(3)	2.9(2)	3.0(2)	2.6(2)	0.1(2)	0.8(2)	-0.1(2)	2.8(1)
C(21)	4.6(3)	2.6(2)	3.3(2)	-0.3(2)	2.0(2)	-0.1(2)	3.4(1)
C(22)	5.6(3)	4.2(3)	4.3(3)	-1.4(3)	1.6(3)	-1.6(3)	4.8(2)
C(23)	7.2(4)	4.5(3)	6.1(3)	-1.2(3)	2.9(3)	-1.6(3)	5.9(2)
C(24)	9.3(4)	3.8(3)	5.5(3)	-0.3(3)	3.4(3)	-0.5(3)	6.0(2)
C(25)	9.7(4)	3.7(3)	4.8(3)	1.4(3)	3.1(3)	0.4(3)	5.8(2)
C(26)	7.4(4)	3.1(3)	4.0(3)	1.6(3)	2.4(2)	0.7(2)	4.6(2)
C(31)	3.3(2)	3.4(2)	2.6(2)	0.4(2)	0.7(2)	-0.1(2)	3.1(1)
C(32)	4.0(3)	3.3(3)	3.8(2)	0.1(2)	1.9(2)	0.4(2)	3.6(1)
C(33)	6.2(3)	3.8(3)	4.3(3)	0.7(3)	2.1(2)	0.6(2)	4.6(2)
C(34)	7.2(4)	5.7(4)	4.2(3)	1.6(3)	2.3(3)	1.3(3)	5.4(2)
C(35)	6.3(4)	8.2(4)	4.2(3)	2.1(4)	1.0(3)	1.5(3)	6.1(2)
C(36)	4.5(3)	6.5(4)	2.9(3)	1.1(3)	0.3(2)	0.5(3)	4.7(2)
C(40)	2.4(2)	3.3(2)	4.1(3)	0.5(2)	1.0(2)	0.3(2)	3.2(1)
C(41)	2.9(2)	3.6(3)	2.3(2)	0.5(2)	0.7(2)	-0.3(2)	2.9(1)
C(42)	3.2(2)	3.9(3)	2.7(2)	-0.5(2)	1.1(2)	-0.6(2)	3.3(1)

Table of General Temperature Factor Expressions - B's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
C(43)	3.2(2)	5.7(3)	3.3(3)	-0.1(2)	1.1(2)	-0.8(2)	4.1(1)
C(44)	2.9(3)	7.9(4)	3.3(3)	0.6(3)	0.6(2)	-0.7(3)	4.7(2)
C(45)	3.5(3)	7.1(4)	4.3(3)	1.7(3)	1.4(2)	0.6(3)	4.8(2)
C(46)	3.5(3)	5.6(3)	3.4(3)	1.6(2)	0.8(2)	0.2(2)	4.2(2)
C(51)	2.4(2)	3.8(2)	2.4(2)	0.5(2)	1.0(2)	0.7(2)	2.8(1)
C(52)	2.9(2)	3.6(3)	3.3(2)	0.3(2)	1.0(2)	1.1(2)	3.2(1)
C(53)	3.8(3)	5.1(3)	5.2(3)	0.8(2)	2.4(2)	1.8(3)	4.4(2)
C(54)	4.6(3)	5.4(3)	5.9(3)	1.3(3)	3.2(2)	2.0(3)	4.9(2)
C(55)	3.7(3)	4.9(3)	4.5(3)	0.9(2)	2.2(2)	1.5(2)	4.1(1)
C(56)	2.9(2)	3.6(3)	2.5(2)	0.7(2)	0.8(2)	0.6(2)	3.0(1)
C(61)	1.9(2)	2.6(2)	3.0(2)	0.1(2)	0.8(2)	-0.5(2)	2.5(1)
C(62)	2.5(2)	2.5(2)	3.0(2)	0.1(2)	1.3(2)	-0.1(2)	2.6(1)
C(63)	3.0(2)	3.2(3)	3.7(2)	0.0(2)	1.3(2)	-0.6(2)	3.3(1)
C(64)	3.0(2)	3.8(3)	3.9(3)	-0.2(2)	1.3(2)	-0.8(2)	3.6(1)
C(65)	2.6(2)	3.6(3)	3.6(2)	0.3(2)	1.1(2)	-0.8(2)	3.3(1)
C(66)	2.2(2)	3.1(2)	2.7(2)	0.5(2)	0.9(2)	-0.1(2)	2.6(1)
C(521)	3.1(2)	2.8(2)	4.9(3)	0.0(2)	1.5(2)	1.1(2)	3.5(1)
C(522)	3.4(3)	3.5(3)	6.3(3)	0.4(2)	1.3(2)	1.5(2)	4.3(2)
C(523)	3.9(3)	3.7(3)	8.3(4)	0.7(2)	2.0(3)	1.6(3)	5.2(2)
C(524)	5.9(3)	4.1(3)	8.4(4)	0.7(3)	3.9(3)	1.3(3)	5.7(2)
C(525)	6.6(3)	3.5(3)	7.9(4)	0.1(3)	4.3(3)	0.8(3)	5.6(2)
C(526)	5.2(3)	3.3(3)	5.0(3)	-0.2(2)	2.6(2)	0.3(2)	4.3(2)
C(561)	3.0(2)	3.3(2)	2.5(2)	0.6(2)	0.9(2)	0.1(2)	2.9(1)

Table of General Temperature Factor Expressions - B's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
C(562)	3.7(2)	3.5(3)	3.2(2)	1.2(2)	1.1(2)	0.5(2)	3.4(1)
C(563)	4.4(3)	3.9(3)	4.3(3)	1.1(2)	1.5(2)	0.6(2)	4.1(1)
C(564)	4.8(3)	3.6(3)	4.7(3)	0.5(2)	1.9(2)	0.2(2)	4.3(2)
C(565)	4.5(3)	3.5(3)	3.4(3)	0.4(2)	1.3(2)	-0.5(2)	3.8(1)
C(566)	3.3(2)	3.4(2)	2.9(2)	0.2(2)	1.1(2)	-0.4(2)	3.2(1)
C(621)	2.7(2)	3.0(2)	3.2(2)	0.3(2)	1.3(2)	0.6(2)	2.9(1)
C(622)	2.5(2)	3.4(2)	3.3(2)	0.0(2)	1.1(2)	0.5(2)	3.0(1)
C(623)	3.2(2)	4.2(3)	4.0(3)	0.7(2)	1.2(2)	1.4(2)	3.7(1)
C(624)	4.5(3)	4.9(3)	4.4(3)	1.4(3)	1.5(2)	1.2(3)	4.4(2)
C(625)	6.1(3)	4.1(3)	4.8(3)	2.0(3)	2.1(3)	1.3(2)	4.7(2)
C(626)	4.8(3)	3.1(3)	4.3(3)	1.0(2)	1.8(2)	0.8(2)	3.9(1)
C(661)	2.1(2)	3.6(2)	2.7(2)	0.7(2)	0.2(2)	0.3(2)	2.8(1)
C(662)	3.1(2)	4.7(3)	3.0(2)	0.7(2)	0.9(2)	0.9(2)	3.5(1)
C(663)	4.7(3)	4.6(3)	4.2(3)	0.6(3)	0.8(2)	1.3(2)	4.4(2)
C(664)	4.6(3)	4.8(3)	4.4(3)	0.3(3)	0.1(3)	1.6(3)	4.7(2)
C(665)	4.2(3)	3.8(3)	4.6(3)	0.7(2)	0.1(3)	0.7(2)	4.3(2)
C(666)	3.2(2)	2.9(2)	4.0(3)	0.9(2)	0.3(2)	0.4(2)	3.4(1)
C(701)	7.0(4)	6.0(4)	11.2(6)	-2.7(4)	2.4(4)	-2.3(4)	8.3(3)
C(702)	7.4(4)	9.2(6)	11.5(6)	-3.1(4)	4.8(4)	-3.5(5)	9.4(3)
C(703)	11.8(7)	11.4(7)	7.7(5)	-2.9(6)	3.2(5)	-1.5(5)	10.4(3)
C(704)	10.1(6)	7.8(5)	6.6(4)	0.7(5)	2.9(4)	1.1(4)	8.0(3)
C(705)	7.7(5)	4.6(3)	7.0(4)	0.8(3)	1.2(4)	0.8(3)	6.4(2)
C(706)	7.1(4)	4.0(3)	8.6(5)	-0.8(3)	0.8(4)	-1.3(4)	6.8(2)

The form of the anisotropic thermal parameter is:

$\exp[-0.25\{h^2a^2B(1,1) + k^2b^2B(2,2) + l^2c^2B(3,3) + 2hkabB(1,2) + 2hlacB(1,3) + 2klbcB(2,3)\}]$ where a, b, and c are reciprocal lattice constants.

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Ti	O(5)	1.816(2)	N(1)	C(2)	1.277(3)
Ti	O(6)	1.829(2)	N(4)	C(3)	1.466(3)
Ti	N(1)	1.910(2)	N(4)	C(40)	1.464(4)
Ti	N(4)	1.886(2)	C(2)	C(3)	1.529(4)
O(5)	C(51)	1.356(3)	C(2)	C(21)	1.487(4)
O(6)	C(61)	1.355(3)	C(3)	C(31)	1.529(4)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(21)	C(22)	1.410(4)	C(44)	C(45)	1.397(5)
C(21)	C(26)	1.400(4)	C(45)	C(46)	1.395(5)
C(22)	C(23)	1.409(5)	C(51)	C(52)	1.400(4)
C(23)	C(24)	1.401(6)	C(51)	C(56)	1.403(4)
C(24)	C(25)	1.402(6)	C(52)	C(53)	1.391(4)
C(25)	C(26)	1.411(5)	C(52)	C(521)	1.484(4)
C(31)	C(32)	1.397(4)	C(53)	C(54)	1.395(5)
C(31)	C(36)	1.395(4)	C(54)	C(55)	1.385(4)
C(32)	C(33)	1.404(4)	C(55)	C(56)	1.405(4)
C(33)	C(34)	1.384(5)	C(56)	C(561)	1.488(4)
C(34)	C(35)	1.389(5)	C(61)	C(62)	1.400(4)
C(35)	C(36)	1.416(5)	C(61)	C(66)	1.395(4)
C(40)	C(41)	1.522(4)	C(62)	C(63)	1.396(4)
C(41)	C(42)	1.389(4)	C(62)	C(621)	1.486(4)
C(41)	C(46)	1.396(4)	C(63)	C(64)	1.398(4)
C(42)	C(43)	1.414(4)	C(64)	C(65)	1.388(4)
C(43)	C(44)	1.399(5)	C(65)	C(66)	1.399(4)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(66)	C(661)	1.486(4)	C(623)	C(624)	1.399(4)
C(521)	C(522)	1.402(4)	C(624)	C(625)	1.396(5)
C(521)	C(526)	1.404(4)	C(625)	C(626)	1.394(4)
C(522)	C(523)	1.407(5)	C(661)	C(662)	1.399(4)
C(523)	C(524)	1.401(5)	C(661)	C(666)	1.412(4)
C(524)	C(525)	1.391(5)	C(662)	C(663)	1.399(4)
C(525)	C(526)	1.399(5)	C(663)	C(664)	1.386(5)
C(561)	C(562)	1.400(4)	C(664)	C(665)	1.403(5)
C(561)	C(566)	1.396(4)	C(665)	C(666)	1.394(4)
C(562)	C(563)	1.396(4)	C(701)	C(702)	1.384(8)
C(563)	C(564)	1.388(5)	C(701)	C(706)	1.371(7)
C(564)	C(565)	1.402(4)	C(702)	C(703)	1.464(8)
C(565)	C(566)	1.390(4)	C(703)	C(704)	1.412(7)
C(621)	C(622)	1.403(4)	C(704)	C(705)	1.374(6)
C(621)	C(626)	1.404(4)	C(705)	C(706)	1.385(6)
C(622)	C(623)	1.408(4)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
O(5)	Ti	O(6)	124.10(8)	Ti	N(4)	C(3)	118.8(2)
O(5)	Ti	N(1)	113.61(9)	Ti	N(4)	C(40)	123.1(2)
O(5)	Ti	N(4)	108.71(9)	C(3)	N(4)	C(40)	118.0(2)
O(6)	Ti	N(1)	114.72(9)	N(1)	C(2)	C(3)	117.9(2)
O(6)	Ti	N(4)	104.27(9)	N(1)	C(2)	C(21)	122.2(3)
N(1)	Ti	N(4)	81.9(1)	C(3)	C(2)	C(21)	119.9(3)
Ti	O(5)	C(51)	161.5(2)	N(4)	C(3)	C(2)	103.5(2)
Ti	O(6)	C(61)	151.5(2)	N(4)	C(3)	C(31)	112.0(2)
Ti	N(1)	C(2)	117.2(2)	C(2)	C(3)	C(31)	111.9(2)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(2)	C(21)	C(22)	121.2(3)	C(40)	C(41)	C(42)	122.1(3)
C(2)	C(21)	C(26)	117.6(3)	C(40)	C(41)	C(46)	117.5(3)
C(22)	C(21)	C(26)	121.1(3)	C(42)	C(41)	C(46)	120.2(3)
C(21)	C(22)	C(23)	118.7(3)	C(41)	C(42)	C(43)	120.4(3)
C(22)	C(23)	C(24)	120.3(4)	C(42)	C(43)	C(44)	118.9(3)
C(23)	C(24)	C(25)	120.9(3)	C(43)	C(44)	C(45)	120.6(3)
C(24)	C(25)	C(26)	119.2(4)	C(44)	C(45)	C(46)	120.0(3)
C(21)	C(26)	C(25)	119.9(3)	C(41)	C(46)	C(45)	120.0(3)
C(3)	C(31)	C(32)	120.8(2)	O(5)	C(51)	C(52)	119.5(2)
C(3)	C(31)	C(36)	119.3(3)	O(5)	C(51)	C(56)	119.0(2)
C(32)	C(31)	C(36)	119.9(3)	C(52)	C(51)	C(56)	121.5(2)
C(31)	C(32)	C(33)	120.3(3)	C(51)	C(52)	C(53)	118.8(3)
C(32)	C(33)	C(34)	119.8(3)	C(51)	C(52)	C(521)	122.0(2)
C(33)	C(34)	C(35)	120.5(3)	C(53)	C(52)	C(521)	119.2(3)
C(34)	C(35)	C(36)	120.1(3)	C(52)	C(53)	C(54)	120.4(3)
C(31)	C(36)	C(35)	119.4(3)	C(53)	C(54)	C(55)	120.5(3)
N(4)	C(40)	C(41)	114.5(2)	C(54)	C(55)	C(56)	120.4(3)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(51)	C(56)	C(55)	118.3(3)	C(522)	C(521)	C(526)	119.4(3)
C(51)	C(56)	C(561)	122.5(2)	C(521)	C(522)	C(523)	119.6(3)
C(55)	C(56)	C(561)	119.0(3)	C(522)	C(523)	C(524)	120.4(3)
O(6)	C(61)	C(62)	119.2(2)	C(523)	C(524)	C(525)	120.0(3)
O(6)	C(61)	C(66)	118.9(2)	C(524)	C(525)	C(526)	119.8(3)
C(62)	C(61)	C(66)	121.8(2)	C(521)	C(526)	C(525)	120.8(3)
C(61)	C(62)	C(63)	117.8(3)	C(56)	C(561)	C(562)	118.7(3)
C(61)	C(62)	C(621)	122.4(2)	C(56)	C(561)	C(566)	122.4(3)
C(63)	C(62)	C(621)	119.5(2)	C(562)	C(561)	C(566)	118.9(3)
C(62)	C(63)	C(64)	121.0(3)	C(561)	C(562)	C(563)	120.3(3)
C(63)	C(64)	C(65)	120.3(3)	C(562)	C(563)	C(564)	120.5(3)
C(64)	C(65)	C(66)	119.8(3)	C(563)	C(564)	C(565)	119.4(3)
C(61)	C(66)	C(65)	119.3(3)	C(564)	C(565)	C(566)	120.0(3)
C(61)	C(66)	C(661)	119.9(2)	C(561)	C(566)	C(565)	120.8(3)
C(65)	C(66)	C(661)	120.7(2)	C(62)	C(621)	C(622)	122.7(2)
C(52)	C(521)	C(522)	119.6(3)	C(62)	C(621)	C(626)	118.3(3)
C(52)	C(521)	C(526)	121.0(3)	C(622)	C(621)	C(626)	119.0(3)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(621)	C(622)	C(623)	120.3(3)	C(663)	C(664)	C(665)	120.2(3)
C(622)	C(623)	C(624)	120.1(3)	C(664)	C(665)	C(666)	120.2(3)
C(623)	C(624)	C(625)	119.5(3)	C(661)	C(666)	C(665)	119.7(3)
C(624)	C(625)	C(626)	120.5(3)	C(702)	C(701)	C(706)	119.8(5)
C(621)	C(626)	C(625)	120.6(3)	C(701)	C(702)	C(703)	120.1(5)
C(66)	C(661)	C(662)	119.5(2)	C(702)	C(703)	C(704)	117.9(5)
C(66)	C(661)	C(666)	120.9(2)	C(703)	C(704)	C(705)	119.1(5)
C(662)	C(661)	C(666)	119.6(3)	C(704)	C(705)	C(706)	122.3(4)
C(661)	C(662)	C(663)	120.2(3)	C(701)	C(706)	C(705)	120.7(5)
C(662)	C(663)	C(664)	120.1(3)				

Numbers in parentheses are estimated standard deviations in the least significant digits.