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Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distancei	ADC
H(7)	H(24)	3.37	66602	H(7)	H(23)	3.52	66602
H(8)	H(17)	2.81	55601	H(8)	H(28)	2.83	65602
H(8)	H(29)	2.89	65602	H(8)	H(16)	3.00	55601
H(8)	H(30)	3.35	65602	H(8)	H(18)	3.52	55601
H(9)	H(20)	2.71	55601	H(9)	H(17)	3.22	55601
H(9)	H(21)	3.28	55601	H(9)	H(16)	3.53	55601
H(10)	H(30)	2.51	65602	H(10)	H(44)	2.65	55601
H(10)	H(43)	3.04	55601	H(10)	H(28)	3.12	65602
H(10)	H(45)	3.18	55601	H(10)	H(29)	3.26	65602
H(11)	H(44)	2.73	55601	H(11)	H(45)	3.33	55601
H(11)	H(41)	3.40	55601	H(12)	H(20)	2.89	55601
H(12)	H(21)	3.06	55601	H(12)	H(19)	3.17	66602
H(12)	H(19)	3.29	55601	H(12)	H(24)	3.53	66602
H(13)	H(23)	2.46	66602	H(13)	H(19)	2.52	66602
H(13)	H(37)	3.06	56602	H(13)	H(20)	3.14	66602
H(13)	H(24)	3.30	66602	H(13)	H(38)	3.50	56602
H(14)	H(15)	3.00	56602	H(14)	H(37)	3.16	56602
H(14)	H(14)	3.39	56602	H(14)	H(42)	3.55	56602
H(15)	H(23)	3.04	45501	H(15)	H(41)	3.17	55601
H(15)	H(40)	3.54	55601	H(15)	H(22)	3.56	45501
H(16)	H(29)	3.40	65502	H(17)	H(25)	3.00	55401
H(17)	H(32)	3.08	65502	H(17)	H(38)	3.19	65501
H(17)	H(29)	3.44	65502	H(18)	H(18)	2.69	65502
H(18)	H(29)	2.83	65502	H(18)	H(32)	3.27	65502

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Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distancei	ADC
H(19)	H(38)	3.55	65501	H(20)	H(38)	2.69	65501
H(22)	H(41)	3.56	65601	H(23)	H(37)	3.03	65501
H(23)	H(39)	3.17	65501	H(23)	H(38)	3.53	65501
H(24)	H(24)	3.39	66602	H(25)	H(33)	2.80	65602
H(25)	H(31)	3.30	65602	H(25)	H(32)	3.59	65602
H(26)	H(33)	2.95	65602	H(26)	H(41)	2.98	65601
H(26)	H(31)	3.15	65602	H(26)	H(36)	3.22	65602
H(26)	H(34)	3.33	65501	H(26)	H(39)	3.34	65501
H(27)	H(41)	2.70	65601	H(27)	H(42)	3.28	65601
H(28)	H(28)	2.71	65602	H(28)	H(33)	3.18	65602
H(29)	H(43)	3.13	65502	H(30)	H(35)	2.75	65501
H(30)	H(43)	3.15	65502	H(30)	H(36)	3.32	65602
H(30)	H(33)	3.33	65602	H(30)	H(34)	3.59	65501
H(31)	H(31)	3.11	2	H(31)	H(35)	3.21	2
H(32)	H(35)	3.05	2	H(34)	H(36)	2.96	55602
H(34)	H(44)	3.03	55601	H(34)	H(34)	3.55	55602
H(34)	H(35)	3.57	55602	H(35)	H(43)	3.05	2
H(35)	H(44)	3.17	2	H(35)	H(36)	3.36	55602
H(36)	H(36)	3.12	55602	H(36)	H(44)	3.13	2
Ru(1)	H(1)	1.67(6)	1	Ru(2)	H(1)	1.89(6)	1

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ± 4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	X,	Y,	Z	(2)	-X,	-Y,	-Z

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Special Contacts

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
Ru(1)	H(1)	1.67(6)	1	Ru(2)	H(1)	1.89(6)	1

Contacts out to 2.05 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one digit numbers and one two digit number: TA(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & TC are the crystal lattice translation digits along cell edges a, b, and c. A translation digit of 5 indicates the origin unit cell. If TA=4, this indicates a translation of one unit cell length along the a axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus (+/-)4 lattice translations from the origin (TA=5,TB=5,TC=5) can be represented.

The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (i.e.cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	+X	,	+Y	,	+Z	(2)	-X	,	-Y	,	-Z