Table 2.1a. Summary table of Format No. 0 ORTEP-III instructions and Format No. 1 instruction continuation cards.

Function	1-3	4-9	10-18	19-27	28-36	37-45	46-54	55-63	64-72
Structure Analysis									
Distances	0, 1, or 2	101	Org. ADR (f)	Org. ADR (t)	Tar. ANR (f)	Tar. ANR (t)	D_{max} (Å)	—	—
(Format No. 1 trailer card)	2	—	—	[LOGC]	—	—	—	—	—
Distances + angles	0, 1, or 2	102	(same as 101)						
Principal axes	—	103	—	—	—	—	—	—	—
Distances single convolute	0, 1, or 2	105	Org. NR (f)	Org. NR (t)	Tar. NR (f)	Tar. NR (t)	D_{max} (Å)	NR Type	—
(Format No. 1 trailer card)	2	—	—	[LOGC]	—	—	—	—	—
Dist. reiterate convolute	0, 1, or 2	106	(same as 105)						
Plotter Control									
Initialize	—	201	—	—	—	—	—	—	—
Shift plot origin/terminate	—	202	[X (in.)]	[Y (in.)]	—	—	—	—	—
Color	—	204	ICOLOR	—	—	—	—	—	—
Pen width	—	205	WIDTH	—	—	—	—	—	—
Drawing Parameters									
Dimensions and view	—	301	X (in.)	Y (in.)	VIEW (in.)	BRDR (in.)	—	—	—
Title rotation	—	302	THETA (°)	—	—	—	—	—	—
Retrace displace	—	303	DISP (in.)	—	—	—	—	—	—
Ellipse smoothness	—	304	CHORD	—	—	—	—	—	—
ATOMS Array									
Run add	0 or 1	401	FROM (1)	(-) TO (1)	[FROM (2)	(-) TO (2)]	[FROM (3)	(-) TO (3)]	…
Run subtract	0 or 1	411	(same as 401)						
Sphere add	0, 1, or 2	402	Org. ADR (f)	Org. ADR (t)	Tar. ANR (f)	Tar. ANR (t)	D_{max} (Å)	—	—
(Format No. 1 trailer card)	2	—	—	[LOGC]	—	—	—	—	—
Sphere subtract	0, 1, or 2	412	(same as 402)						
Box add	0, 1, or 2	403	Org. ADR (f)	Org. ADR (t)	Tar. ANR (f)	Tar. ANR (t)	a/2 (Å)	b/2 (Å)	c/2 (Å)
(Format No. 1 trailer card)	2	—	—	[LOGC]	—	—	—	—	—
Box subtract	0, 1, or 2	413	(same as 403)						
Triclinic box add	0, 1, or 2	404	Org. ADR (f)	Org. ADR (t)	Tar. ANR (f)	Tar. ANR (t)	a/2 (fract.)	b/2 (fract.)	c/2 (fract.)
(Format No. 1 trailer card)	2	—	—	[LOGC]	—	—	—	—	—
Triclinic box subtract	0, 1, or 2	414	(same as 404)						
Convolute add	0, 1, or 2	405	Org. NR (f)	Org. NR (t)	Tar. NR (f)	Tar. NR (t)	D_{max} (Å)	NR Type	—
(Format No. 1 trailer card)	2	—	—	[LOGC]	—	—	—	—	—
Convolute subtract	0, 1, or 2	415	(same as 405)						
Reiterate convolute add	0, 1, or 2	406	Org. NR (f)	Org. NR (t)	Tar. NR (f)	Tar. NR (t)	D_{max} (Å)	NR Type	—
(Format No. 1 trailer card)	2	—	[ASYMUNIT]	[LOGC]	—	—	—	—	—
Reiterate convolute subt.	0, 1, or 2	416	(same as 406)						
Zero ATOMS array	—	410	—	—	—	—	—	—	—

Table 2.1a. Summary table of Format No. 0 ORTEP-III instructions and Format No. 1 instruction continuation cards.

Function	1-3	4-9	10-18	19-27	28-36	37-45	46-54	55-63	64-72
Cartesian System									
Explicit definition	—	501	ORGN	V1 (f)	V1 (t)	V2 (f)	V2 (t)	—	Type
Rotate reference	0 or 1	502	Axis No.	Rotation (°)	[Axis No.	Rotation]	…	…	…
Rotate working	—	503	Axis No.	Rotation (°)	—	—	—	—	—
Translate reference	—	504	ΔX (in.)	ΔY (in.)	ΔZ (in.)	—	—	—	—
Origin at centroid	0 or 2	505	—	—	—	—	—	—	—
Centroid org./inertial axes	0 or 2	506	—	—	—	—	—	—	—
Position and Scale									
Explicit center and scale	—	601	X0 (in.)	Y0 (in.)	SCAL1	SCAL2*	—	—	—
Explicit center and auto scale	—	602	X0 (in.)	Y0 (in.)	—	SCAL2*	—	—	—
Explicit scale and auto center	—	603	—	—	SCAL1	SCAL2*	—	—	—
Auto center and scale	—	604	—	—	—	SCAL2*	—	—	—
Incr. position and incr. scale	—	611	ΔX0 (in.)	ΔY0 (in.)	ΔSCAL1	SCAL2*	—	—	—
Incr. position and auto scale	—	612	ΔX0 (in.)	ΔY0 (in.)	—	SCAL2*	—	—	—
Incr. scale and auto center	—	613	—	—	ΔSCAL1	SCAL2*	—	—	—
Atom Plotting									
Shaded octant football	0 or 1	701	—	—	—	—	Sym. hgt. (in.)	∥ Offset (in.)	⊥ Offset (in.)
(Format No. 1 trailer card)	—	—	A0 (in.)	A1 (in.)	NR (f)	NR (t)	NR Type	—	—
Football	0 or 1	702	(same as 701)						
Open model	0 or 1	703	(same as 701)						
Boundary only	0 or 1	704	(same as 701)						
Explicit ellipsoid description	0 or 1	705	NPLANE	NDOT	NLINE	NDASH	Sym. hgt. (in.)	∥ Offset (in.)	⊥ Offset (in.)
(Format No. 1 trailer card)	—	—	A0 (in.)	A1 (in.)	NR (f)	NR (t)	NR Type	—	—
Open octant football	0 or 1	706	(same as 701)						
As above except	0 or 1	711	(same as 701)						
no printed output of	0 or 1	712	(same as 701)						
individual coordinates	0 or 1	713	(same as 701)						
	0 or 1	714	(same as 701)						
	0 or 1	715	(same as 705)						
	0 or 1	716	(same as 701)						

*Or probability (entered as negative whole number).

Table 2.1a. Summary table of Format No. 0 ORTEP-III instructions and Format No. 1 instruction continuation cards.

Function	1-3	4-9	10-18	19-27	28-36	37-45	46-54	55-63	64-72
Bond Plotting									
Explicit	[1 &] 2	801	ADC (f)	ADC (t)	[ADC (f)	ADC (t)]	[ADC (f)	ADC (t)]	…
Implicit stick	2	802	—	NR Type	—	—	—	—	—
Implicit line	2	803	—	NR Type	—	—	—	—	—
As above except	[1 &] 2	811	(same as 801)						
no printed output	2	812	(same as 802)						
	2	813	(same as 803)						
Label Plotting									
Atom label	—	901	ADC 1	[ADC 2]	X Reset (in.)	Y Reset (in.)	HGT (in.)	∥ Offset (in.)	⊥ Offset (in.)
Regular title	3	902	ADC 1	[ADC 2]	X Reset (in.)	Y Reset (in.)	HGT (in.)	∥ Offset (in.)	⊥ Offset (in.)
Normal plane vector title	3	903	ADC 1	ADC 2	X Reset (in.)	Y Reset (in.)	HGT (in.)	∥ Offset (in.)	⊥ Offset (in.)
General plane vector title	3	913	ADC 1	ADC 2	—	—	HGT (in.)	∥ Offset (in.)	⊥ Offset (in.)
Nrm. plane bond-length label									
(1 decimal place)	—	904	ADC 1	ADC 2	X Reset (in.)	Y Reset (in.)	HGT (in.)	∥ Offset (in.)	⊥ Offset (in.)
(2 decimal places)	—	905	(same as 904)						
(3 decimal places)	—	906	(same as 904)						
Gen. plane bond-length label									
(1 decimal place)	—	914	ADC 1	ADC 2	—	—	HGT (in.)	∥ Offset (in.)	⊥ Offset (in.)
(2 decimal places)	—	915	(same as 914)						
(3 decimal places)	—	916	(same as 914)						
Overlap Correction									
Atoms [and implicit bonds]	0 [or 2]	1001	0, 1, or	NR Type	—	—	—	—	—
(Format No. 1 trailer card)			OVMRGN (in.)						
Explicit bonds	[1 &] 2	821	ADC (f)	ADC (t)	[ADC (f)	ADC (t)]	[ADC (f)	ADC (t)]	…
Implicit bonds	2	822	—	NR Type	—	—	—	—	—
Save Sequence									
Start	—	1101	—	—	—	—	—	—	—
End	—	1102	—	—	—	—	—	—	—
Execute	—	1103	—	—	—	—	—	—	—
Terminate	—	-1	—	—	—	—	—	—	—
Next Structure	—	-2	—	—	—	—	—	—	—

Table 2.1b. Summary table of Format No. 2 instruction continuation cards.

				Positive Number or Blank in Col. 43-48			Negative Number in Col. 43-48	
Columns	101,102,105, 106,402/412, 405/415, 406/416	403/413, 404/414	505,506	801/811,821	802/812,822,1001	803/813	802/812, 822,1001	803/813
3	0 or 2	0 or 2	0 or 2	0 or 2	0 or 2	0 or 2	0 or 2	0 or 2
4-9	—	—	—	—	—	—	—	—
10-12	[Org. NR (f)	[Org. NR (f)	NR (f)	—	Org. NR (f)	Org. NR (f)	Org. NR (f)	Org. NR (f)
13-15	Org. NR (t)]	Org. NR (t)]	NR (t)	—	Org. NR (t)	Org. NR (t)	Org. NR (t)	Org. NR (t)
16-18	[Tar. NR (f)	[Tar. NR (f)	—	—	Tar. NR (f)	Tar. NR (f)	Tar. NR (f)	Tar. NR (f)
19-21	Tar. NR (t)]	Tar. NR (t)]	—	—	Tar. NR (t)	Tar. NR (t)	Tar. NR (t)	Tar. NR (t)
22-24	[NR type]	NR type	NR type	Bond type	Bond type	—	Bond type	—
25-30	[D_{min} (Å)	—	Weight	—	D_{min} (Å)	D_{min} (Å)	D_{min} (Å)	D_{min} (Å)
31-36	D_{max} (Å)]	—	—	—	D_{max} (Å)	D_{max} (Å)	D_{max} (Å)	D_{max} (Å)
37-42	—	—	—	Bond radius (Å)	Bond radius (Å)	—	Bond radius (Å)	—
43-48	—	—	—	Persp. label hgt. (in.)	Persp. label hgt. (in.)	—	Poly. NR (f)	Poly. NR (f)
49-54	—	—	—	⊥ displacement (in.)	⊥ displacement (in.)	—	Poly. NR (t)	Poly. NR (t)
55-60	—	—	—	Nonp. label hgt. (in.)	Nonp. label hgt. (in.)	—	Poly. D_{min} (Å)	Poly. D_{min} (Å)
61-66	—	—	—	⊥ displacement (in.)	⊥ displacement (in.)	—	Poly. D_{max} (Å)	Poly. D_{max} (Å)
67-72	—	—	—	Digits indicator	Digits indicator	—	—	—