SUPPLEMENTARY DATA (10 Pages) Acta Crystallographica Section B

Automated Assignment of Graph Set Descriptors for Crystallographically-Symmetric Molecules.

W. D. SAMUEL MOTHERWELL,* GREGORY P. SHIELDS AND FRANK H. ALLEN

Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, U.K.

E-mail: motherwell@ccdc.cam.ac.uk

Abstract

Algorithms for the automatic assignment of graph set notation for intermolecular networks have been extended to molecules having internal crystallographic symmetry, for patterns up to second level. This provides a means of achieving systematic and consistent assignments for networks containing symmetric molecules. These methodologies have been implemented in the program RPLUTO. Examples are given of the application of the method to a number of molecules with H-bonded and other intermolecular networks, illustrating the diversity of patterns which occur.

Supplementary Table

Graph Set assignments for selected CSD structures
(contacts are N/O-H...N/O H-bonds unless otherwise indicated).

(a) *One independent H-edge*		
CSD Refcode	a>	a>a<
BAFXEC	**S**1,1(6)	
	S2,2(10)	
BASVUM01	**S**1,1(6)	
	S2,2(14)	
BOCNEM	**S**1,1(6)	
	S2,2(16)	
DLACAM10	**S**1,1(5)	
	S2,2(10)	
SILTUC01	**S**1,1(5)	
	S2,2(14)	
VEHZEN, VEHZIR, VEHZIR01, WIDBIU	**S**1,1(5) **S**3,3(15)	
YIRYAZ	**S**1,1(8)	
	S3,3(12)	
	S3,3(24)	
HIWQEJ	**S**3,3(6)	
	S1,1(4)	
	S3,3(12)	
KUWWUV	**S**1,1(8)	
	S3,3(30)	
	S3,3(24)	
FESCAH CH...O	**S**1,1(5)	
	S3,3(9)	
	S3,3(15)	
KIVDOI	**C**1,1(4)	**C**1,2(6)
NUTTIF	**C**1,1(4)	**C**1,2(6)
TETSSU Te...O	**C**1,1(4)	**C**2,1(8)
EIMCAM10	**C**1,1(6)	**C**2,2(18)
	C1,1(9)	
FALRIT	**C**1,1(2)	**C**2,2(16)
	C1,1(8)	
GLOXIM	**C**1,1(3)	**C**2,2(12)
	C1,1(6)	
KOSZAT	**C**1,1(5)	**C**2,2(12)
	C1,1(6)	
ZEHFIB	**C**1,1(2)	**C**2,2(14)
	C1,1(7)	
PAPSII,	**C**1,1(2)	**C**2,2(16)

PAPSOO, POKVUG, ZAZROH,	**C**1,1(8)	
	ZAZSOI, ZAZTAV, ZAZTID, ZAZTOJ, ZAZTUP	
SILTUC01	**C**1,1(4)	**R**1,2(6)
TIDGUI	**C**1,1(2)	**R**2,1(4)
CEJTUG	**C**1,1(4)	**R**2,2(12)
	C1,1(5)	
JOFHER	**C**1,1(4)	**R**2,2(12)
	C1,1(6)	
YUZPAK	**C**1,1(4)	**R**2,2(16)
	C1,1(8)	
PELBIR	**C**1,1(2)	**C**2,2(16)
	C1,1(8)	**R**6,6(48)
KELCAF	**R**4,4(12)	**R**2,2(10)
	R4,4(20)	
BAFTAD10	**R**6,6(12)	**R**2,2(16)
	R2,2(16)	
	R6,6(48)	
RUHWUM	**R**2,2(22)	**C**2,2(22)
	R6,6(30)	**R**6,6(66)
	R6,6(66)	
TEPHTH	**C**1,1(9)	**R**2,2(18)
	R2,2(8)	
BASVUM01	**C**1,1(6)	**C**2,2(16)
	R6,6(42)	
BOLNOF	**C**1,1(6)	**C**2,2(18)
	R4,4(36)	
FAXHOB01	**C**1,1(2)	**C**2,2(14)
	R4,4(28)	
HIKNOE	**C**1,1(9)	**C**2,2(8)
	R6,6(12)	
HYQUIN05, JAMKEN, ZZZVLG01	**C**1,1(7)	**C**2,2(14)
	R6,6(12)	
MMALAC01	**C**1,1(6)	**C**2,2(12)
	R2,2(8)	
NIMGOF	**C**1,1(2)	**C**2,2(14)
	R4,4(28)	
SEPCUL	**C**1,1(7)	**C**2,2(14)
	R2,2(12)	
ZALVEN	**C**1,1(4)	**C**2,2(16)
	R2,2(16)	
FESCAH	**C**1,1(5)	**C**2,2(10)
CH...O	**C**3,3(9)	**R**6,6(30)
	R3,3(15)	
GEJVEW	**C**1,1(8)	**C**2,2(16)

	R2,2(8)	**R**8,8(64)
GESTAZ	**C**1,1(8)	**C**2,2(16)
	R2,2(8)	**R**8,8(64)
PERYTO03	**C**1,1(6)	**C**2,2(12)
	R4,4(8)	**R**4,4(24)
	R2,2(12)	**R**8,8(48)
	R4,4(24)	
FETRUR	**D**1,1(2)	
GEMBEF	**D**1,1(2)	**D**2,2(19)
HIMGAL	**D**1,1(2)	**D**2,2(9)
HMTTPO10	**D**1,1(2)	**D**2,2(5)
PIPEDC10	**D**1,1(2)	**D**2,2(10)
BOCNEM	**D**1,1(2)	**C**1,2(8)
KOMRUZ	**D**1,1(2)	**C**2,2(16)
YOHNOY	**D**1,2(2)	**C**1,2(7)
JASXUW	**D**1,1(2)	**R**1,2(7)
BOLDIP10	**D**1,1(2)	**C**1,2(6)
		C2,2(6)
		C2,2(8)
		R2,2(8)
		R3,6(12)
		R4,4(16)
		R3,6(18)
		R6,6(18)
		R6,6(24)
HIFZIF	**D**1,1(2)	**C**2,2(18)
		R6,6(54)
NUNSIY01	**D**1,1(2)	**C**2,2(6)
CH...O		**C**2,2(8)
		R1,2(6)
		R2,4(8)
		R2,4(12)
		R4,4(16)
		R8,8(24)
		R8,8(32)
TAMGUC01	**D**1,1(2)	**C**1,2(6)
		R3,6(18)
WIDBIU	**D**1,1(2)	**C**2,2(12)
		R6,6(36)

(b) *Two independent H-edges*

	a>	**a**>**a**<	**b**>	**b**>**b**<	**a**>**b**>	**a**<**b**>
HMTETZ10	**S**1,1(6)		**S**1,1(5)			
	S2,2(10)		**S**2,2(12)			

ALOXAN	**C**1,1(4)	**C**1,2(6)	**C**1,1(4) **C**1,1(6)	**C**2,2(10)	**C**2,2(10) **R**2,2(8) **R**4,4(16) **R**4,4(20)	**C**2,1(6) **C**2,2(10)
HAGPUA	**C**1,1(7) **C**1,1(8)	**C**2,2(16)	**C**1,1(8) **C**1,1(9)	**C**2,2(18)	**C**2,2(15) **C**2,2(16) **C**2,2(17)	**C**2,2(17) **R**2,1(5) **R**4,4(20) **R**4,2(24)
JALHIN	**C**1,1(4) **C**1,1(10)	**C**2,2(20) **R**6,6(60)	**C**1,1(4) **C**1,1(10)	**C**2,2(20) **R**6,6(20)	**C**2,2(8) **C**2,2(14) **C**2,2(20)	**C**1,2(12) **C**2,2(12) **R**3,6(12) **R**2,2(20) **R**3,6(36) **R**6,6(36) **R**6,6(60)
GOHREA04 B...Cl	**C**1,1(2) **C**1,1(4)	**C**2,2(8) **R**6,6(24)	**C**1,1(3) **C**1,1(5)	**C**2,2(8) **C**6,6(24)	**C**2,2(7) **C**2,2(9) **R**2,2(5) **R**6,6(15) **R**6,6(21) **R**6,6(27)	**C**2,1(5) **C**2,1(7) **C**2,2(7) **C**2,2(9)
MERYOL03	**C**1,1(2) **R**4,4(28)	**C**2,2(14)	**C**1,1(5) **R**4,4(8)	**C**2,2(10)	**C**2,2(11) **R**2,2(11) **R**4,4(20) **R**4,4(24)	**C**2,2(10) **C**2,2(11) **C**2,2(12) **R**4,4(24)
UREAXX	**C**1,1(4) **R**4,4(16)	**C**1,2(6)	**C**1,1(4)	**R**1,2(6)	**C**2,2(8) **R**8,8(32)	**C**1,2(4) **C**1,2(6) **R**4,8(16) **R**4,8(24)
YISTEZ	**D**1,1(2)	**D**2,2(10)	**D**1,1(2)	**D**2,2(8)	**C**2,2(6) **C**2,2(11)	
BOLDIP	**D**1,1(2)	**C**2,2(8) **R**6,6(24)	**D**1,1(2)	**C**2,2(8) **R**6,6(24)		**C**1,2(6) **C**2,2(6) **R**2,2(8) **R**3,6(12) **R**3,6(18) **R**6,6(18) **R**6,6(24)
EAMNIB CH...O	**D**1,1(2)	**C**2,2(8) **R**2,2(8) **R**8,8(32)	**D**1,1(2)	**C**2,2(14) **R**8,8(56)		**C**2,2(9) **C**2,2(11) **R**4,4(14) **R**4,4(22)

HIWQEJ OH...F	**D**1,1(2)	**C**2,2(8)	**D**1,1(2)	**C**2,2(8)		**C**2,1(4) **C**2,2(8) **R**6,3(12)
ZUKKAR	**D**1,1(2)	**C**2,2(30)	**D**1,1(2)	**C**2,2(30)	**C**2,2(8) **R**2,2(30) **R**4,4(38)	
EXPORD10	**D**1,1(2)	**C**2,2(14) **R**8,8(40)	**D**1,1(2)	**R**1,2(12) **R**4,8(32)	**C**2,2(7) **C**2,2(11) **R**4,4(14) **R**4,4(22)	
AMTBTZ NH...Cl	**D**1,1(2)	**R**1,2(8) **R**2,4(16)	**D**1,1(2)	**C**1,2(8) **R**2,4(16)		**D**2,2(5) **D**2,2(9)
VOBXEP	**D**1,1(2)	**R**1,2(10)	**D**1,1(2)	**C**2,2(12)		**D**2,2(5) **D**2,2(11)
TUQNEY	**D**1,2(2)	**C**1,2(6) **C**2,2(6) **C**2,2(8) **R**2,2(8) **R**3,6(12) **R**4,4(16) **R**3,6(18) **R**6,6(18) **R**6,6(24)	**D**1,1(2)	**C**1,2(6) **C**2,2(6) **C**2,2(8) **R**2,2(8) **R**3,6(12) **R**4,4(16) **R**3,6(18) **R**6,6(18) **R**6,6(24)		**D**2,2(6)
YINJOU	**D**1,1(2)	**D**2,2(13)	**C**1,1(10) **R**2,2(8)	**C**2,2(20) **R**8,8(80)	**C**2,3(16) **C**3,3(32)	
SAKYOS10	**R**6,6(12)		**D**1,1(2)	**D**2,2(5)	**C**3,3(8)	
HMTAAB	**D**1,1(2)		**D**1,1(2)	**C**2,2(6) **R**6,6(18)		**C**2,2(6)

(c) *Three independent H-edges*

------	**a**> **a**>**b**>	**a**>**a**< **a**>**b**<	**b**> **a**>**c**>	**b**>**b**< **a**>**c**<	**c**> **b**>**c**>	**c**>**c**< **b**>**c**<
YIRYIH	**S**1,1(8) **S**3,3(12) **S**3,3(24)		**S**1,1(5) **S**3,3(21)		**S**1,1(11) **S**3,3(15) **S**3,3(33)	
ETDAMS ------	**D**1,1(2)	**C**2,2(9) **C**1,2(4) **C**2,2(6) **C**1,2(7) **C**2,2(9)	**D**1,1(2)	**C**2,2(9) **C**2,2(6) **C**2,2(9)	**D**1,1(2)	**R**2,2(9) **C**2,2(6) **C**2,2(9)
BUYSET10 ------	**C**1,1(7)		**D**1,1(2)	**D**2,2(7)	**C**1,1(6)	

	C3,3(17)		**C**2,2(7)	**C**2,2(13)	**C**3,3(14)	
HMTETZ10 ------	**R**4,4(8)		**D**1,1(2)		**D**1,1(2)	**D**2,2(12)
	C3,3(13)		**C**2,3(13)		**C**2,2(7) **R**8,8(32)	
VOJFEF ------	**D**1,1(2)	**D**2,2(23)	**D**1,1(2)	**D**2,2(23)	**D**1,1(2)	**D**2,2(21)
		D1,2(3) **D**2,2(23)	**D**2,2(6) **D**2,2(22)		**R**2,2(8) **R**4,4(48) **R**8,8(96)	

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