

ELECTRONIC SUPPLEMENTARY INFORMATION

Advancing the use of Voronoi–Dirichlet polyhedra to describe interactions in organic molecular crystal structures by the example of galunisertib polymorphs

Viktor N. Serezhkin,* Anton V. Savchenkov

Samara National Research University, Samara, Russian Federation

* *E-mail:* serezhkin@samsu.ru

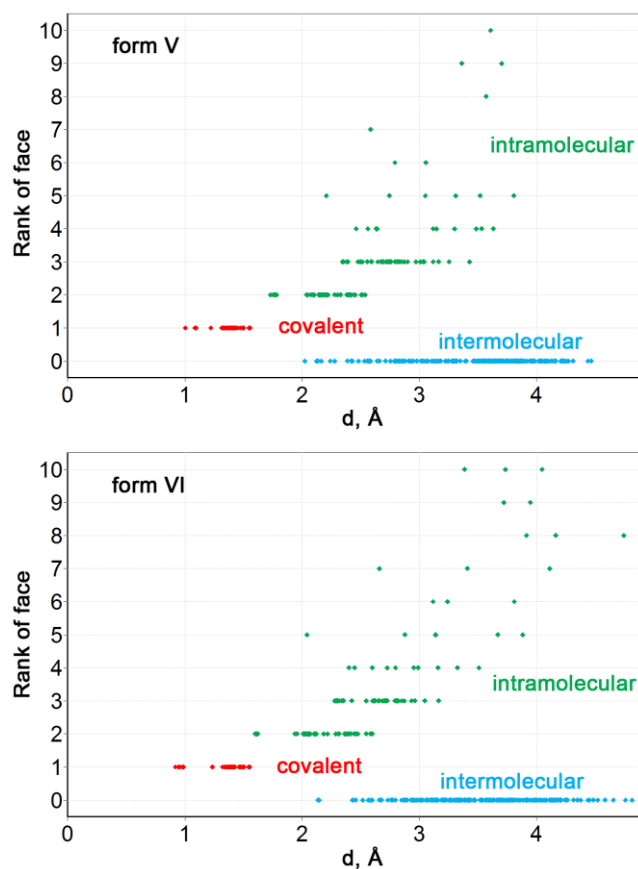


Fig. S1. (RF, d) distributions for molecular VD polyhedra of GAL molecules with the same 1k values equal to 246: form V (top) and form VI (bottom).

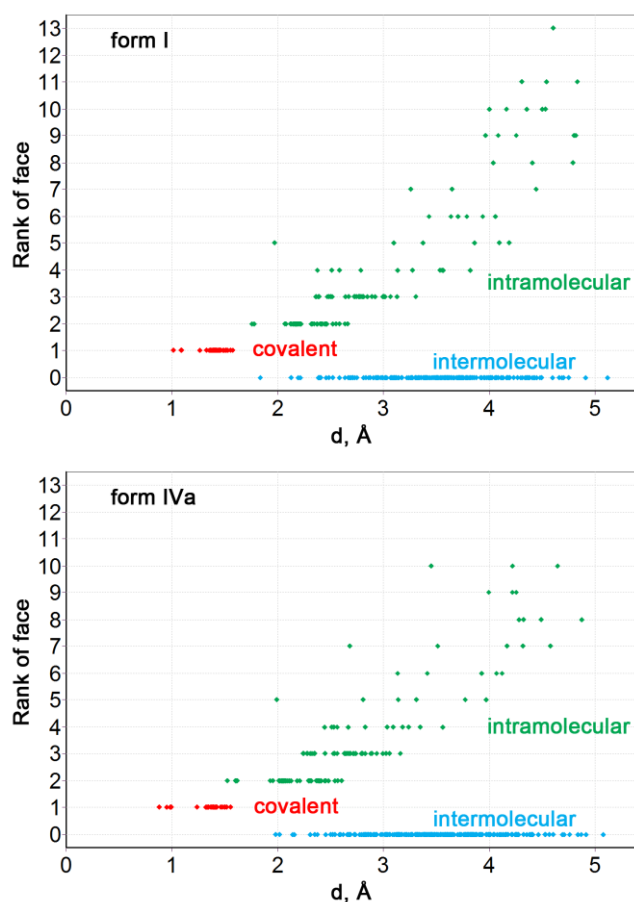


Fig. S2. (RF, d) distributions for molecular VD polyhedra of GAL molecules with the same 1k values equal to 272: form I (top) and form IVa (bottom).

The following Tables S1–S3 include these characteristics of atomic interactions:

- k – the number of pyramids representing interatomic contacts;
- d_{\min} and d_{\max} (Å) – distances for the shortest and the longest contact respectively;
- S (Å²) – the total surface area of all faces corresponding to the given type of contacts;
- V (Å³) – the total volume of all pyramids corresponding to the given type of contacts;
- Δ_S (%) – partial contributions of contacts to the total surface area of the corresponding faces.

The last column Σ shows the cumulative values for each molecule.

Table S1. Characteristics of chemical bonds in GAL polymorphs (VD polyhedra faces with RF = 1)

Form	Refcode		H/C	C/C	H/N	C/N	N/N	C/O	Σ
I	DORDUM09	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.09	1.39	1.01	1.33	1.35	1.26	1.01
		d_{\max}	1.09	1.58	1.02	1.46	1.35	1.26	1.58
		<i>S</i>	193.38	301.27	22.84	104.73	14.20	14.09	650.52
		<i>V</i>	35.09	72.39	3.87	23.90	3.20	2.96	141.40
		Δ_S	29.73	46.31	3.51	16.10	2.18	2.17	100.00
II	DORDUM	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.36	0.88	1.31	1.35	1.23	0.88
		d_{\max}	0.99	1.55	0.88	1.48	1.35	1.23	1.55
		<i>S</i>	187.31	286.41	24.72	100.58	11.87	14.49	625.38
		<i>V</i>	30.07	67.76	3.63	22.66	2.68	2.97	129.75
		Δ_S	29.95	45.80	3.95	16.08	1.90	2.32	100.00
III	DORDUM01	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.36	0.88	1.32	1.35	1.24	0.88
		d_{\max}	0.99	1.55	0.88	1.46	1.35	1.24	1.55
		<i>S</i>	183.04	280.90	24.82	103.74	12.68	14.14	619.32
		<i>V</i>	29.39	66.41	3.64	23.35	2.85	2.91	128.55
		Δ_S	29.55	45.36	4.01	16.75	2.05	2.28	100.00
IV	DORDUM02	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.36	0.88	1.32	1.34	1.24	0.88
		d_{\max}	0.99	1.55	0.88	1.46	1.35	1.24	1.55
		<i>S</i>	181.22	283.40	24.71	103.19	13.31	13.65	619.48
		<i>V</i>	29.11	67.15	3.62	23.24	2.98	2.82	128.92
		Δ_S	29.25	45.75	3.99	16.66	2.15	2.20	100.00
	IVa	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.37	0.88	1.32	1.35	1.24	0.88
		d_{\max}	0.99	1.55	0.88	1.46	1.35	1.24	1.55
		<i>S</i>	183.79	289.34	27.33	105.21	13.40	13.49	632.56
		<i>V</i>	29.51	68.51	4.01	23.68	3.01	2.78	131.50
		Δ_S	29.05	45.74	4.32	16.63	2.12	2.13	100.00
	IVb	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.36	0.88	1.32	1.34	1.24	0.88
		d_{\max}	0.99	1.54	0.88	1.46	1.34	1.24	1.54
		<i>S</i>	178.66	277.46	22.09	101.16	13.22	13.81	606.40
		<i>V</i>	28.70	65.79	3.24	22.80	2.96	2.85	126.34
		Δ_S	29.46	45.76	3.64	16.68	2.18	2.28	100.00
V	DORDUM03	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.08	1.37	1.01	1.32	1.32	1.22	1.01
		d_{\max}	1.10	1.55	1.01	1.45	1.32	1.22	1.55
		<i>S</i>	189.29	290.95	22.62	99.98	13.24	15.32	631.40
		<i>V</i>	34.35	69.15	3.79	22.50	2.92	3.12	135.83
		Δ_S	29.98	46.08	3.58	15.84	2.10	2.43	100.00
VI	DORDUM04	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.36	0.92	1.32	1.35	1.23	0.92
		d_{\max}	0.99	1.55	0.96	1.46	1.35	1.23	1.55
		<i>S</i>	185.48	281.89	21.07	96.48	13.50	14.25	612.67
		<i>V</i>	29.78	66.82	3.30	21.75	3.04	2.93	127.61
		Δ_S	30.27	46.01	3.44	15.75	2.20	2.33	100.00

Table S1 (continued)

Form	Refcode		H/C	C/C	H/N	C/N	N/N	C/O	Σ
VII	DORDUM10	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.06	1.35	1.00	1.29	1.31	1.22	1.00
		d_{\max}	1.11	1.55	1.03	1.43	1.32	1.23	1.55
		<i>S</i>	189.96	278.72	23.02	100.47	13.74	13.71	619.61
		<i>V</i>	34.20	65.40	3.87	22.34	3.01	2.80	131.61
		Δ_S	30.66	44.98	3.71	16.22	2.22	2.21	100.00
	VIIa	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.06	1.35	1.00	1.29	1.32	1.23	1.00
		d_{\max}	1.11	1.55	1.02	1.43	1.32	1.23	1.55
		<i>S</i>	187.78	285.26	22.74	100.44	13.39	12.90	622.51
		<i>V</i>	33.75	66.95	3.82	22.33	2.95	2.64	132.44
		Δ_S	30.16	45.82	3.65	16.13	2.15	2.07	100.00
	VIIb	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.07	1.36	1.00	1.31	1.31	1.22	1.00
		d_{\max}	1.11	1.53	1.03	1.42	1.31	1.22	1.53
<i>S</i>		192.13	272.18	23.29	100.50	14.08	14.52	616.70	
<i>V</i>		34.64	63.85	3.93	22.34	3.07	2.95	130.79	
Δ_S		31.16	44.13	3.78	16.30	2.28	2.35	100.00	
VIII	DORDUM05	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.06	1.35	1.03	1.33	1.35	1.27	1.03
		d_{\max}	1.10	1.53	1.03	1.42	1.35	1.27	1.53
		<i>S</i>	179.61	275.37	22.90	98.75	11.62	15.21	603.45
		<i>V</i>	32.51	64.87	3.92	22.12	2.61	3.21	129.24
		Δ_S	29.76	45.63	3.79	16.36	1.92	2.52	100.00
IX	DORDUM06	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	1.08	1.37	1.00	1.32	1.33	1.22	1.00
		d_{\max}	1.10	1.55	1.01	1.45	1.33	1.22	1.55
		<i>S</i>	192.75	283.11	27.18	99.73	13.61	17.08	633.46
		<i>V</i>	34.98	67.23	4.56	22.44	3.01	3.48	135.69
		Δ_S	30.43	44.69	4.29	15.74	2.15	2.70	100.00
X	DORDUM07	<i>k</i>	34	44	4	16	2	2	102
		d_{\min}	0.95	1.37	0.88	1.32	1.35	1.25	0.88
		d_{\max}	0.99	1.55	0.88	1.46	1.35	1.25	1.55
		<i>S</i>	176.76	272.12	23.48	99.22	14.01	12.12	597.70
		<i>V</i>	28.39	64.46	3.44	22.31	3.16	2.53	124.28
		Δ_S	29.57	45.53	3.93	16.60	2.34	2.03	100.00

Table S2. Characteristics of intramolecular noncovalent interactions in GAL polymorphs (VD polyhedra faces with RF > 1)

Form	Refcode		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	Σ
I	DORDUM09	<i>k</i>	52	122	34	32	26		4	2		272
		d_{\min}	1.76	2.07	2.32	2.08	2.12		2.51	2.42		1.76
		d_{\max}	4.83	4.82	3.31	4.80	3.43		2.52	2.42		4.83
		<i>S</i>	125.56	81.57	5.45	50.75	16.89		8.52	0.04		288.78
		<i>V</i>	46.79	38.31	2.30	22.80	8.20		3.56	0.02		121.98
		Δ_S	43.48	28.25	1.89	17.57	5.85		2.95	0.01		100.00
II	DORDUM	<i>k</i>	52	116	44	24	26		4	2		268
		d_{\min}	1.52	1.93	2.22	1.94	2.13		2.44	2.37		1.52
		d_{\max}	4.32	4.68	3.20	3.83	3.82		2.48	2.37		4.68
		<i>S</i>	155.09	82.09	3.90	34.09	11.94		13.76	0.41		301.26
		<i>V</i>	57.08	36.43	1.55	14.60	5.59		5.67	0.16		121.07
		Δ_S	51.48	27.25	1.29	11.31	3.96		4.57	0.13		100.00
III	DORDUM01	<i>k</i>	50	118	44	24	26		4	2		268
		d_{\min}	1.52	1.93	2.21	1.95	2.11		2.44	2.36		1.52
		d_{\max}	4.09	4.63	5.10	4.50	3.25		2.46	2.36		5.10
		<i>S</i>	128.09	84.19	5.47	35.09	13.39		9.62	0.89		276.75
		<i>V</i>	46.82	38.39	2.69	14.68	6.47		3.94	0.35		113.33
		Δ_S	46.29	30.42	1.98	12.68	4.84		3.48	0.32		100.00
IV	DORDUM02	<i>k</i>	50	114	45	28	25		5	3		270
		d_{\min}	1.52	1.93	2.21	1.95	2.11		2.45	2.37		1.52
		d_{\max}	4.65	4.88	4.58	4.22	4.07		3.65	2.80		4.88
		<i>S</i>	130.23	73.77	4.17	35.83	14.66		11.30	0.42		270.37
		<i>V</i>	46.06	32.41	1.77	14.81	7.02		4.85	0.17		107.09
		Δ_S	48.17	27.28	1.54	13.25	5.42		4.18	0.16		100.00
	IVa	<i>k</i>	50	114	46	30	26		4	2		272
		d_{\min}	1.52	1.93	2.21	1.95	2.11		2.45	2.38		1.52
		d_{\max}	4.65	4.88	4.58	4.22	4.07		2.51	2.38		4.88
		<i>S</i>	130.32	67.46	4.34	30.62	14.78		9.90	0.44		257.86
		<i>V</i>	46.65	29.37	1.92	12.71	7.22		4.13	0.17		102.15
		Δ_S	50.54	26.16	1.68	11.87	5.73		3.84	0.17		100.00
	IVb	<i>k</i>	50	114	44	26	24		6	4		268
		d_{\min}	1.52	1.93	2.21	1.95	2.11		2.45	2.37		1.52
		d_{\max}	4.04	3.73	3.32	2.92	3.08		3.65	2.80		4.04
		<i>S</i>	130.13	80.07	4.00	41.04	14.54		12.70	0.41		282.88
		<i>V</i>	45.47	35.46	1.61	16.92	6.83		5.57	0.16		112.02
		Δ_S	46.00	28.30	1.41	14.51	5.14		4.49	0.14		100.00

Table S2 (continued)

Form	Refcode		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	Σ
V	DORDUM03	k	46	104	42	26	20		4	4		246
		d_{\min}	1.73	2.04	2.21	2.05	2.10		2.50	2.38		1.73
		d_{\max}	3.61	3.80	3.43	3.04	3.12		2.56	2.87		3.80
		S	95.31	60.67	4.07	45.67	10.27		10.75	1.03		227.77
		V	36.57	25.54	1.64	19.31	4.79		4.56	0.41		92.82
		Δ_S	41.84	26.64	1.79	20.05	4.51		4.72	0.45		100.00
VI	DORDUM04	k	50	102	38	26	24		4	2		246
		d_{\min}	1.60	1.94	2.22	1.96	2.11		2.42	2.37		1.60
		d_{\max}	4.05	4.74	3.17	3.74	3.67		2.45	2.37		4.74
		S	124.89	75.53	3.24	34.81	13.20		12.72	0.26		264.66
		V	44.33	33.12	1.30	15.17	6.26		5.17	0.10		105.46
		Δ_S	47.19	28.54	1.22	13.15	4.99		4.81	0.10		100.00
VII	DORDUM10	k	50	106	39	26	20	1	4	3	1	250
		d_{\min}	1.72	2.00	2.18	2.03	2.09	2.68	2.35	2.33	2.22	1.72
		d_{\max}	4.39	4.19	3.71	3.43	3.00	2.68	2.49	2.78	2.22	4.39
		S	112.47	62.81	3.92	29.77	6.68	1.73	10.07	1.07	<0.01	228.52
		V	42.12	26.13	1.58	12.12	2.87	0.78	4.09	0.43	<0.01	90.12
		Δ_S	49.22	27.48	1.71	13.03	2.92	0.76	4.41	0.47	<0.01	100.00
	VIIa	k	48	104	38	24	18	2	4	2	2	242
		d_{\min}	1.72	2.00	2.26	2.03	2.09	2.68	2.35	2.33	2.22	1.72
		d_{\max}	3.57	4.13	3.71	3.43	2.73	2.68	2.44	2.33	2.22	4.13
		S	112.41	68.19	4.11	24.98	2.87	3.47	8.88	0.22	<0.01	225.14
		V	41.24	28.54	1.67	9.93	1.08	1.55	3.52	0.09	<0.01	87.62
		Δ_S	49.93	30.29	1.83	11.10	1.27	1.54	3.95	0.10	<0.01	100.00
	VIIb	k	52	108	40	28	22		4	4		258
		d_{\min}	1.73	2.03	2.18	2.06	2.09		2.47	2.34		1.73
		d_{\max}	4.39	4.19	2.75	3.43	3.00		2.49	2.78		4.39
		S	112.54	57.42	3.72	34.56	10.50		11.26	1.92		231.90
		V	43.00	23.72	1.50	14.30	4.67		4.66	0.78		92.63
		Δ_S	48.53	24.76	1.60	14.90	4.53		4.86	0.83		100.00
VIII	DORDUM05	k	48	102	40	20	22		4	2	2	240
		d_{\min}	1.76	2.02	2.22	2.05	2.12		2.40	2.39	2.26	1.76
		d_{\max}	4.20	4.02	3.60	3.15	3.30		2.50	2.39	2.26	4.20
		S	104.52	55.66	5.03	32.89	10.20		13.05	0.40	0.55	222.28
		V	40.08	23.16	2.02	13.71	4.79		5.31	0.16	0.21	89.43
		Δ_S	47.02	25.04	2.26	14.80	4.59		5.87	0.18	0.25	100.00

Table S2 (continued)

Form	Refcode		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	Σ
IX	DORDUM06	k	52	104	44	28	22		4	2		256
		d_{\min}	1.72	2.03	2.21	2.05	2.10		2.42	2.37		1.72
		d_{\max}	4.08	3.73	3.45	3.41	3.50		2.47	2.37		4.08
		S	125.96	60.96	3.61	32.80	9.07		9.77	0.58		242.74
		V	46.37	25.72	1.47	14.12	4.33		3.97	0.23		96.21
		Δ_S	51.89	25.11	1.49	13.51	3.74		4.02	0.24		100.00
X	DORDUM07	k	48	112	36	28	20		4	2		250
		d_{\min}	1.52	1.93	2.21	1.95	2.13		2.42	2.38		1.52
		d_{\max}	3.56	4.25	2.99	3.66	3.17		2.44	2.38		4.25
		S	118.51	69.17	3.66	43.69	12.82		11.11	0.12		259.08
		V	41.94	29.46	1.45	18.36	6.16		4.49	0.05		101.90
		Δ_S	45.74	26.70	1.41	16.86	4.95		4.29	0.05		100.00

Table S3. Characteristics of intermolecular noncovalent interactions in GAL polymorphs (VD polyhedra faces with RF = 0)

Form	Refcode		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	Σ
I	DORDUM09	<i>k</i>	129	118	35	50	12	6	18	4			372
		<i>d</i> _{min}	2.12	2.83	3.58	2.41	3.38	3.80	1.84	3.53			1.84
		<i>d</i> _{max}	5.12	4.60	4.42	4.91	4.43	4.12	3.51	3.70			5.12
		<i>S</i>	235.21	107.78	10.82	68.10	7.43	3.52	35.55	0.05			468.46
		<i>V</i>	113.46	60.07	7.17	34.88	4.34	2.30	15.62	0.03			237.87
		Δ_S	50.21	23.01	2.31	14.54	1.59	0.75	7.59	0.01			100.00
II	DORDUM	<i>k</i>	134	136	27	42	16	3	14	4			376
		<i>d</i> _{min}	2.42	2.73	3.54	2.21	3.44	3.47	2.01	4.21			2.01
		<i>d</i> _{max}	6.26	5.91	4.30	4.00	3.99	3.49	4.06	4.50			6.26
		<i>S</i>	238.79	106.39	11.91	64.74	6.97	2.13	36.60	1.96			469.48
		<i>V</i>	135.82	59.73	7.34	30.38	4.21	1.23	16.40	1.38			256.49
		Δ_S	50.86	22.66	2.54	13.79	1.48	0.45	7.80	0.42			100.00
III	DORDUM01	<i>k</i>	126	150	12	48	16		14	4			370
		<i>d</i> _{min}	2.32	2.69	3.65	2.64	3.60		2.06	3.15			2.06
		<i>d</i> _{max}	4.78	4.66	4.09	4.61	4.36		3.34	3.23			4.78
		<i>S</i>	214.27	115.61	3.59	74.64	6.07		36.68	0.89			451.74
		<i>V</i>	108.10	63.96	2.29	37.34	3.78		16.44	0.47			232.38
		Δ_S	47.43	25.59	0.79	16.52	1.34		8.12	0.20			100.00
IV	DORDUM02	<i>k</i>	124	170	11	44	17	4	14	6			389
		<i>d</i> _{min}	2.31	2.68	3.55	2.14	3.43	3.39	1.98	3.85			1.98
		<i>d</i> _{max}	5.08	4.92	4.76	4.28	4.11	3.97	4.53	4.87			5.08
		<i>S</i>	217.91	120.97	3.49	63.16	5.92	3.42	35.84	2.69			453.39
		<i>V</i>	110.73	67.76	2.26	30.84	3.71	2.01	15.42	1.83			234.55
		Δ_S	48.06	26.68	0.77	13.93	1.31	0.75	7.91	0.59			100.00
	IVa	<i>k</i>	125	165	12	41	16	5	18	12			394
		<i>d</i> _{min}	2.31	2.68	3.55	2.14	3.43	3.39	1.98	3.85			1.98
		<i>d</i> _{max}	5.08	4.92	4.76	4.21	4.11	3.97	4.53	4.87			5.08
		<i>S</i>	217.53	121.26	4.25	57.50	5.30	4.28	45.97	5.37			461.45
		<i>V</i>	109.61	68.62	2.73	26.93	3.26	2.56	19.95	3.67			237.32
		Δ_S	47.14	26.28	0.92	12.46	1.15	0.93	9.96	1.16			100.00
	IVb	<i>k</i>	123	175	9	47	18	2	10				384
		<i>d</i> _{min}	2.31	2.68	3.93	2.14	3.43	3.39	1.98				1.98
		<i>d</i> _{max}	5.08	4.71	4.45	4.28	4.11	3.58	3.43				5.08
		<i>S</i>	218.28	120.67	2.73	68.81	6.54	2.56	25.72				445.31
		<i>V</i>	111.85	66.89	1.79	34.76	4.16	1.46	10.89				231.80
		Δ_S	49.02	27.10	0.61	15.45	1.47	0.57	5.78				100.00

Table S3 (continued)

Form	Refcode		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	Σ
V	DORDUM03	k	132	132	50	36	34	6	22	10			422
		d_{\min}	2.12	2.76	3.61	2.28	3.40	3.68	2.02	3.74			2.02
		d_{\max}	4.44	4.46	4.24	4.16	3.95	4.02	4.21	4.26			4.46
		S	240.94	88.47	18.03	46.32	24.10	0.84	38.44	3.95			461.08
		V	110.82	50.02	11.28	23.79	14.46	0.52	17.66	2.50			231.05
		Δ_S	52.25	19.19	3.91	10.05	5.23	0.18	8.34	0.86			100.00
VI	DORDUM04	k	127	166	8	38	14	3	16	2	4		378
		d_{\min}	2.43	2.76	3.81	2.14	3.54	3.69	2.43	3.43	3.44		2.14
		d_{\max}	4.81	4.58	4.21	3.95	4.17	3.75	4.76	3.43	3.61		4.81
		S	216.63	132.69	0.57	62.72	5.68	1.34	34.57	0.63	2.98		457.80
		V	111.38	74.80	0.39	28.60	3.44	0.83	16.59	0.36	1.78		238.17
		Δ_S	47.32	28.98	0.12	13.70	1.24	0.29	7.55	0.14	0.65		100.00
VII	DORDUM10	k	125	151	41	51	13	5	14	5	1	1	406
		d_{\min}	2.10	2.51	3.46	2.10	3.33	3.25	2.08	3.55	3.90	3.09	2.08
		d_{\max}	5.02	4.61	4.71	4.16	4.14	3.86	4.89	4.35	3.90	3.09	5.02
		S	218.70	113.05	15.07	64.66	5.34	5.39	35.51	2.55	0.23	0.70	461.20
		V	104.35	61.40	9.55	30.61	3.20	3.17	15.62	1.57	0.15	0.36	229.99
		Δ_S	47.42	24.51	3.27	14.02	1.16	1.17	7.70	0.55	0.05	0.15	100.00
	VIIa	k	126	148	41	52	11	5	15	6	2		406
		d_{\min}	2.10	2.51	2.51	2.11	3.33	3.25	2.08	3.55	3.90		2.08
		d_{\max}	5.02	4.61	4.61	4.16	4.14	3.86	3.74	4.35	3.90		5.02
		S	216.05	112.41	15.06	69.08	5.28	5.62	31.30	4.61	0.46		459.87
		V	101.64	60.51	9.55	32.79	3.17	3.35	15.05	2.83	0.30		229.19
		Δ_S	46.98	24.44	3.27	15.02	1.15	1.22	6.81	1.00	0.10		100.00
	VIIb	k	123	154	41	50	15	5	13	4		1	406
		d_{\min}	2.17	2.51	2.51	2.10	3.33	3.25	2.08	3.56		3.09	2.08
		d_{\max}	4.79	4.61	4.61	4.16	3.98	3.82	4.89	4.35		3.09	4.89
		S	221.36	113.70	15.08	60.24	5.40	5.15	39.72	0.48		1.39	462.52
		V	107.05	62.30	9.56	28.43	3.24	2.99	16.19	0.32		0.72	230.80
		Δ_S	47.86	24.58	3.26	13.02	1.17	1.11	8.59	0.10		0.30	100.00
VIII	DORDUM05	k	122	164	30	42	20	6	14	2			400
		d_{\min}	2.08	2.63	3.23	2.13	3.34	3.35	2.09	3.86			2.08
		d_{\max}	4.71	4.49	3.90	4.08	3.96	4.13	4.02	3.86			4.71
		S	233.60	116.99	10.86	61.65	14.22	2.23	39.95	0.34			479.85
		V	111.68	63.60	6.30	29.39	8.30	1.29	18.98	0.22			239.75
		Δ_S	48.68	24.38	2.26	12.85	2.96	0.46	8.32	0.07			100.00

Table S3 (continued)

Form	Refcode		H/H	H/C	C/C	H/N	C/N	N/N	H/O	C/O	N/O	O/O	Σ
IX	DORDUM06	k	119	148	32	50	20	3	16	4			392
		d_{\min}	2.00	2.57	3.23	2.15	3.24	3.62	2.04	4.08			2.00
		d_{\max}	5.62	4.59	4.39	5.47	4.04	3.81	3.95	4.25			5.62
		S	225.10	122.34	11.38	62.49	15.56	1.88	38.74	0.46			477.94
		V	106.17	69.54	6.63	29.35	8.82	1.14	17.87	0.32			239.84
		Δ_S	47.10	25.60	2.38	13.07	3.26	0.39	8.11	0.10			100.00
X	DORDUM07	k	123	126	48	44	32	6	18			1	398
		d_{\min}	2.37	2.72	3.29	2.40	3.34	3.78	2.00			3.52	2.00
		d_{\max}	4.35	4.14	4.43	4.28	4.14	3.97	4.33			3.52	4.43
		S	220.30	100.59	9.94	46.74	23.20	1.11	39.41			0.01	441.28
		V	108.18	54.64	6.35	22.70	13.49	0.72	17.84			<0,01	223.92
		Δ_S	49.92	22.80	2.25	10.59	5.26	0.25	8.93			<0,01	100.00