

Supplementary Information

Conformer label	$\theta_1 / ^\circ$	$\theta_2 / ^\circ$	Energy / kJmol ⁻¹			Volume per molecule / Å ³	Space group	Packing Motif
			ΔE_{intra}	U_{latt}	E_{tot}			
3a	88	160	13.05	-108.95	-95.90	173.93	P2 ₁ /c	III
3a	88	160	13.05	-108.90	-95.84	173.21	P2 ₁ /c	I
3b	90	160	13.07	-108.81	-95.74	173.36	P2 ₁ /c	I
3b	90	160	13.07	-108.79	-95.72	174.44	P2 ₁ /c	III
3c	90	160	13.30	-108.94	-95.64	173.7	P2 ₁ /c	I
3c	90	160	13.30	-108.88	-95.58	174.76	P2 ₁ /c	III
3d	90	160	12.81	-108.35	-95.53	173.13	P2 ₁ /c	I
3d	90	160	12.81	-108.30	-95.49	174.18	P2 ₁ /c	III
10g	80	160	13.57	-109.03	-95.46	172.58	P2 ₁ /c	III
10g	80	160	13.57	-108.93	-95.37	172.91	P2 ₁ /c	I
3a	88	160	13.05	-108.16	-95.11	172.32	P-1	2
10g	80	160	13.57	-108.66	-95.09	171.5	P-1	2
3e	90	160	12.53	-107.52	-94.99	172.99	P2 ₁ /c	I
3c	90	160	13.30	-108.23	-94.93	175.49	P-1	II
3e	90	160	12.53	-107.36	-94.83	174.03	P2 ₁ /c	III
3c	90	160	13.30	-108.12	-94.83	173.09	P-1	2
3b	90	160	13.07	-107.85	-94.78	172.69	P-1	2
3b	90	160	13.07	-107.85	-94.77	172.69	P-1	2
3a	88	160	13.05	-107.75	-94.70	175.1	P-1	II
3b	90	160	13.07	-107.70	-94.63	175.34	P-1	II
3d	90	160	12.81	-107.27	-94.46	172.4	P-1	2
10g	80	160	13.57	-107.86	-94.29	173.83	P-1	II
3f	90	160	12.27	-106.37	-94.10	173	P2 ₁ /c	I
3d	90	160	12.81	-106.87	-94.06	175.25	P-1	II
10d	100	160	13.71	-107.70	-93.99	174.51	P2 ₁ /c	I
3e	90	160	12.53	-106.37	-93.84	172.27	P-1	2
3f	90	160	12.27	-106.01	-93.74	174.03	P2 ₁ /c	III
10d	100	160	13.71	-107.36	-93.65	175.66	P2 ₁ /c	III
10b	120	-34	12.55	-106.10	-93.56	174.6	P2₁/c	IV
10d	100	160	13.71	-107.08	-93.37	175.88	P-1	II
10g	80	160	13.57	-106.73	-93.16	175.38	P2 ₁ /c	3
3e	90	160	12.53	-105.63	-93.10	175.28	P-1	II
3f	90	160	12.27	-105.26	-92.99	172.47	P-1	2
1d	69	-160	10.81	-103.16	-92.35	176.03	P-1	4
10b	120	-34	12.55	-104.90	-92.35	179.3	P-1	5
3g	90	160	12.10	-104.40	-92.30	173.2	P2 ₁ /c	I
1c	87	160	12.04	-104.19	-92.16	173.02	P2 ₁ /c	I
4b	90	160	19.35	-111.44	-92.09	173.16	P-1	II
1d	69	-160	10.81	-102.75	-91.94	179.07	P2₁/c	6
3c	90	160	13.30	-105.21	-91.91	178.81	P2 ₁ /c	7
1c	87	160	12.04	-103.88	-91.84	172.2	P-1	2
3g	90	160	12.10	-103.88	-91.78	173.04	P-1	2
2a	100	160	12.84	-104.54	-91.71	173.87	P2 ₁ /c	I
2a	100	160	12.84	-104.54	-91.70	173.75	P-1	2
1c	87	160	12.04	-103.68	-91.64	173.95	P2 ₁ /c	III
3g	90	160	12.10	-103.72	-91.63	174.21	P2 ₁ /c	III
2c	80	160	12.37	-103.83	-91.46	170.69	P-1	2
10h	120	-20	13.80	-105.23	-91.43	176.83	P-1	5
4a	90	160	20.37	-111.79	-91.42	172.35	P-1	II
6f	120	-36	12.01	-103.35	-91.34	175.48	P2 ₁ /c	IV
10h	120	-20	13.80	-105.12	-91.32	173.74	P2 ₁ /c	IV
3a	88	160	13.05	-104.31	-91.25	178.04	P2 ₁ /c	7
9o	120	160	15.77	-106.89	-91.12	174.39	P2₁/c	8

10b	120	-34	12.55	-103.66	-91.11	182.41	C2/c	9
3b	90	160	13.07	-104.17	-91.10	178.54	P2 ₁ /c	7
1a	68	-150	11.18	-102.27	-91.09	179.02	P2₁/c	10
4c	90	160	19.27	-110.36	-91.09	173.86	P-1	II
10a	74	-150	14.36	-105.40	-91.05	176.48	P-1	4
1e	96	140	16.24	-107.14	-90.91	175.01	P2 ₁ /c	1

Crystal structures in the lowest 5kJmol⁻¹ of E_{tot}; the six structures in bold were suggested (in the order they appear here) as predictions of form IV.