

A.Gavezzotti

Pillars of crystal engineering

crystal energies and symmetry operators

Electronic supplementary information Part 1

Sublimation enthalpy vs. lattice energy

CSD refcode	SE	LE	delt
ACEMID05	79.1	-74.6	5.7
ACETYL	18.5	-21	-13.5
AHEMAB	117.1	-101.6	13.2
AMIPYR	83	-90.5	-9
AMMTAZ01	92.7	-106.1	-14.5
AMPYRD	78	-83.5	-7
AMPYRE01	88	-96.9	-10.1
APYFEB01	113	-107.6	4.8
ARCLAM01	83.3	-79.8	4.2
AZTHYM10	116.3	-99.4	14.5
BARBAC01	122.9	-106.5	13.3
BDTOLE11	95.9	-83	13.4
BETHAZ01	71	-75.4	-6.3
BEXQOK01	112.1	-121	-8
BIRYIK11	88	-92	-4.6
BISJIW	70.3	-67.3	4.3
BOTYIT	77	-87.3	-13.3
BRANIL	100	-89.7	10.3
BRCYTS	153.5	-139.9	8.9
BRNIBZ	87	-81.8	6
CAACTY	40.5	-38.9	4
CAGPUV01	85	-85	0
CARDOO	109	-106	2.8
CLACET07	82.1	-84.1	-2.5
CLBENQ	68.1	-74.1	-8.7
CLNIBZ01	82	-82.1	-0.1
CLNOAN	109	-103.4	5.2
CLNOBE02	103	-96.4	6.4
CROTAM	82.9	-84.8	-2.3
CUVJUY	102.8	-88.9	13.6
CYANAC	101.7	-107	-5.2
CYANAM01	75.1	-79.2	-5.5
CYAPYR	75	-74	1.4
CYNGEN	29.5	-33.9	-14.9
CYPYRO01	106.8	-91.3	14.6
CYURAC13	133.1	-129.3	2.8
DACETA	73	-80.3	-10
DCLBQN01	70	-76.2	-8.8
DCPYAZ01	70	-79	-12.9
DCYANM	42.9	-39.7	7.4
DIACHZ	105.2	-106.9	-1.6
DIKPIP03	109.2	-123.4	-13
DITHAN03	71	-70.6	0.5
DIXTAF01	88	-86.8	1.4
DLGYAH	84.1	-77.9	7.4

DMEOXA06	75	-70.9	5.4
DTOLTO	82.1	-70.2	14.5
DTURAC01	124.9	-126.4	-1.2
DUCKOB03	28.4	-30	-5.9
ECARBM10	75.1	-80.1	-6.6
FEPGEM	75.1	-75.3	-0.2
FIZZOD	96.1	-86.7	9.8
FORMAC01	59.5	-53.7	9.7
FULPIM	88.6	-87.9	0.8
FUMAAC01	137.9	-124.1	10
FURACL03	133	-113.9	14.3
GEBTUC01	164	-153.9	6.1
GLURAC13	131.1	-127	3.1
GLUTIM	94	-84.5	10.1
HAMGOT	91.8	-94.8	-3.2
HIBWEU	83	-82.5	0.6
HIFKUC	87.1	-89	-2.1
IBURAM	85.9	-82.2	4.4
ISNICA	113	-111.1	1.7
ITIZOA	72.2	-76.7	-6.3
JAHZEX10	130.9	-135	-3.1
KOMYEQ01	80	-72.7	9.2
LAKJEM	86.6	-99	-14.2
LETFEV	73	-75.7	-3.7
LETNAZ01	103	-100.4	2.5
LIJFUG	86	-81.6	5.1
MALIAC13	110.5	-107.3	2.9
MALNAC16	109.5	-101	7.7
MALOAM02	126	-140.9	-11.8
MEMALA01	115	-109.3	4.9
MENPDL	101.7	-100	1.7
METCYT01	159.1	-137.7	13.5
MEUREA01	97.9	-106.3	-8.6
MNIANL11	94	-104.3	-11
MUBZOY	71	-74.7	-5.2
MUBZUE	72	-69.1	4
NANILI31	101	-99.2	1.8
NEPGCL02	87.9	-90.5	-2.9
NICOAC02	124	-107.4	13.4
NIJHJ04	90.1	-94.1	-4.5
NITPOL08	95	-92.1	3
NTCPOL01	88	-83.1	5.6
NTRGUA01	143.1	-150.9	-5.4
OFIZEK	84	-82.4	1.9
ONITPH	73	-66.8	8.5
OWEKEH	73	-68.9	5.5
OXALAC08	95.5	-106.9	-11.9
PBRANL01	79	-88.6	-12.1
PBRPOL	85	-87.1	-2.4
PENTAN01	35.8	-39.4	-10.1
PERYTO13	151.3	-149.4	1.3
PICANO04	97.2	-92.9	4.5
PRONAC	70.8	-66.9	5.5

PTOxec	88	-87.6	0.5
PUVVUZ	89.5	-78.9	11.8
PYRDNO11	79	-83.6	-5.8
PYRZIN23	90.7	-101.7	-12.1
PYRZOL38	73.1	-77.3	-5.7
QOPBED	70.1	-70.6	-0.8
QQQBNG01	74	-76.5	-3.4
QQQCIS01	22.5	-23.5	-4.4
QQQGEM01	103.1	-109.3	-6
RAKSIG	154.5	-167.6	-8.5
SACBAA02	21.8	-22.3	-2.2
SETVIX	81	-76.4	5.7
SSOXAM02	105.3	-110.8	-5.3
SUCACB18	122.1	-112.8	7.6
SUCANH16	82.1	-75.9	7.6
SUCCIN09	86.5	-83.4	3.5
TCBENQ19	100.6	-99.9	0.7
TCYETY11	84	-74.8	11
TELPOP	87.1	-88.6	-1.8
TEMWUD	74	-68.1	8
TETZOL02	90.1	-88.2	2.1
TFACAM	79.1	-72.9	7.9
THACEM01	83.1	-87.6	-5.4
THBARB01	115.3	-107.4	6.8
THIOUR16	109.3	-122.9	-12.4
THYMIN01	133	-114.8	13.7
TOXOCN	80	-79.3	0.9
TPENAC02	97.8	-91.8	6.2
TRAZOL04	82.1	-89	-8.4
TRITAN10	94.1	-89.2	5.2
TRIZIN01	57.1	-59.6	-4.4
TROXAN	56.1	-63	-12.3
TURCIL03	129	-125	3.1
UCAYED01	66.9	-69.9	-4.5
UGUMUE	110.7	-115.7	-4.5
ULEBOD	87	-77.2	11.2
URACIL	131	-114.1	12.9
UREAXX25	98.3	-103.8	-5.7
VOQYUW	82	-74.5	9.1
WIFKEB02	96.1	-101.1	-5.2
XAGWIM02	100.5	-97.3	3.1
YAQLAE	98.1	-109.2	-11.3
YAQLEI	104.9	-118.8	-13.2
YAQZUM	85	-74.6	12.2
YOVCAO	100	-102.4	-2.4
ZILNOX	78	-77.3	0.9
ZUDTID	110.8	-113.2	-2.1
ZZZEKW02	87	-86.3	0.8
ZZZKAY05	79.5	-76.5	3.7
ZZZKDQ01	85.5	-87.9	-2.8
ZZZKJQ01	91.1	-96.5	-6
ZZZVYE01	36	-35.2	2.3
ZZZWEO02	29.9	-28.5	4.7

ADIPAC20	145	-125.7	13.3
AMBACO08	110	-99.8	9.3
AMPHOL01	108.1	-124.2	-14.9
AMPHOM02	101	-114.6	-13.4
BECJEY	90	-83.7	7
BENZAC20	91	-93.1	-2.3
BENZEN18	44.3	-46.2	-4.4
BEOXAZ	65	-60.2	7.4
BESKAL	130	-123.2	5.3
BIDLOP02	123	-115.3	6.2
BIPJUF	135	-116.3	13.9
BNZQUI03	68.8	-59.7	13.3
BRBZAC01	109	-103.1	5.4
BRBZAP01	107	-100.2	6.3
BZAMID12	100.5	-99.1	1.4
BZDMAZ04	100	-100.6	-0.6
BZOXZO	98	-90	8.2
CACDAM01	111	-109.6	1.3
CAJWEQ01	88	-84.8	3.7
CAPLAC	85.5	-81.7	4.5
CBUTAC	112	-112.2	-0.2
CLBZAC02	110	-102.1	7.2
CLBZAP13	105	-104.4	0.6
COVJIG01	94.3	-90.1	4.4
CYHEXO01	84	-73.1	13
DNBENZ15	85	-76.4	10.1
DNITBZ11	95	-84.4	11.2
EHOWIH	115	-110.1	4.3
FACRIK05	90	-89.8	0.2
FBENZA02	94	-90.4	3.8
FECCOF01	110	-117.4	-6.7
FURDCA	124.7	-124.7	0
GOCWEA	82	-79.6	2.9
HEXANE01	46.2	-45.7	1
HXMTAM23	77	-85.4	-10.9
HYQUIN08	100.9	-106.2	-5.2
LEZJAB01	109	-119.8	-9.9
MAMPOL	104	-107.6	-3.4
MCBZAC02	104	-101.1	2.8
MEADEN05	126.1	-135.4	-7.4
NBZOAC12	120	-109.6	8.7
NBZOAO04	119	-109.2	8.2
NICOAM06	120	-112.6	6.2
NITOLU01	77	-67.5	12.3
PHGLOL01	134	-141.1	-5.3
PICAMD06	93.9	-97.2	-3.5
PNBZNT	91	-79.2	13
POKKAB	95	-96.3	-1.3
RAJGUG	89	-78	12.3
RESORA03	93	-100.9	-8.5
RICFEP01	81	-78.8	2.8
SALIAC19	97	-92.1	5
UCOVAL	96	-93.4	2.7

XOGJAG	52.2	-50.2	3.9
YELRIR	89	-94.6	-6.3
YIFZAP	115	-129	-12.1
ZZZDRQ01	85	-80.7	5
ZZZEEU04	125	-121.6	2.7
ZZZFYW02	93	-85.1	8.5
ZZZIVG02	59.8	-63.4	-6
ZZZKAO01	59.9	-61.3	-2.4
ZZZVCO04	83	-80.4	3.2
AMACPH01	93.8	-97.8	-4.3
AMBNAC12	116	-125.7	-8.4
AMEBAC	107	-100.2	6.4
ANISIC04	111	-99.7	10.2
BENZDC11	142	-122.4	13.8
BISJAO02	81	-77.7	4.1
BOXAZD	114	-97.1	14.9
CPXACA01	120	-130.3	-8.6
DAZNAP	82	-92.4	-12.6
DIMEDO02	100	-91.3	8.7
DIMNAN01	102	-92	9.8
DIMPHE12	84.2	-87.1	-3.4
DMADEN11	118.1	-117.9	0.1
DMEPOL10	75.5	-78.8	-4.3
DMKETD02	71	-60.9	14.3
DMPHOL11	85.2	-82.4	3.2
DTENYL02	85.6	-76.8	10.3
FUFBOX	107	-106.1	0.9
HACTPH16	97.5	-89.2	8.5
HEPTAN02	53.4	-51.1	4.3
HEYJOK01	68	-72.9	-7.2
JEXNAB	133	-129	3
LIMLOI	106.9	-91.1	14.8
MBNZAM10	83.5	-93.5	-12
MNTDMA01	93	-83.3	10.5
MOXBEN01	84	-76.9	8.4
MPSUFO01	92	-104.4	-13.4
OBIZEE	90	-79.2	12
OCRSOL02	75	-79.1	-5.5
OTOLIC02	96	-94.1	1.9
PHTHAC06	130	-137.8	-6
PHUREA02	140.3	-131	6.6
PIMELA15	140	-135.9	2.9
PTOLIC01	99	-88.5	10.6
QQQAPG02	40.1	-42.8	-6.8
TEPHTH14	146	-135.6	7.1
TEPNIT11	90	-80.8	10.3
VAYJIO	117.8	-133	-12.9
VIDMAX	125	-127.3	-1.8
WIGYIV	107	-103.5	3.3
YUYPUD02	87	-79.8	8.3
ZBCNON	58	-57.9	0.2
ZZZITY02	58.8	-63.8	-8.5
BIPYRL04	80	-87.8	-9.7

BULVAL03	72	-65.1	9.6
CHLQUI10	84	-94.2	-12.1
CLQUIN	81	-89.5	-10.5
COUMAR02	92.3	-80.4	12.9
DMBNZA11	99	-97	2
DMBZAC01	105	-97.6	7.1
DMOXBA01	122	-133.5	-9.4
DMTPAL	105.2	-93.3	11.3
DURENE	73.1	-67.1	8.2
EYIRIN	102	-105.5	-3.5
FAMDIG	112	-105.3	6
FESNOG02	174.5	-166.9	4.4
HEGFAB	116	-128.3	-10.6
HEKMOZ	127	-115.2	9.3
HXQUIN11	99	-92.1	6.9
IPMEPL	91.1	-85	6.7
ISUQUI	123	-112.4	8.6
ISURAP	116	-99.5	14.2
JIBDON	84	-72	14.3
KEYNOR	87.7	-84.5	3.7
NAPHOL01	90	-97.1	-7.9
NAPHQU01	91	-79.1	13.1
NAPHTA10	73	-74.9	-2.6
NBORAN02	97	-84.2	13.2
NONMEI	93	-99.3	-6.7
NPHHQU10	122.3	-123.4	-0.9
ODOTOQ	93	-84.2	9.4
PICGAJ	109	-111.3	-2.1
REZRIY	98.2	-98.3	-0.1
RUVQAA	110	-100.5	8.7
SECQEY	104	-109.3	-5.1
SUZXOB	94	-88.3	6
UPAJIF	107	-100	6.6
WIZJUL	104	-93.3	10.3
XAXSIY	90	-85.9	4.5
ZZZFLM01	129	-112.3	13
ZZZNCU01	113	-104.1	7.8
CINMAC	107	-103.8	3
MXCINN02	134	-116.5	13.1
OVERAT01	117	-117.8	-0.7
PEXBZA	123	-112	9
TMBZAC01	104	-96.1	7.6
TMEBZA	111	-101.5	8.6
ZZZNRU02	124	-110.8	10.7
AZBENC01	93.1	-93.1	0
BIMVEZ	100	-102.2	-2.2
BIPHEN04	82	-83.9	-2.3
BOPSAA10	110	-118.1	-7.3
BPHENO10	93.1	-87.4	6.1
BZDIOX01	92.1	-85.4	7.3
CONYAH	93.7	-86.6	7.6
CRBZOL03	101	-111.1	-10
DBZFUR02	84.1	-79.9	5

DBZTHP	96.1	-90.6	5.7
DCBDOX10	110.4	-107.5	2.7
DCBZDX20	112.5	-117.5	-4.4
DCLBIP	96	-101	-5.2
DECFDP01	87.1	-75.4	13.4
DMNAPH	81.5	-80.9	0.7
DMNPTL02	83.1	-85.4	-2.9
DOHDPH02	143	-152.5	-6.6
DPSULO	106	-111.7	-5.3
FELSEU	114.7	-127.9	-11.5
FLUREN01	85.1	-81	4.8
HIBXOF	135	-121.4	10.1
NAPACA12	112	-114.3	-2.1
NAPOAC01	115.9	-105.3	9.2
NUTSUQ	114	-121.3	-6.4
OCDBDO10	154.3	-169.7	-10
PARPEE	95	-94.3	0.7
PEYGEF01	124	-124.7	-0.5
PHBENZ01	98	-97.7	0.3
PHENAZ11	96	-92.8	3.3
PHESAZ01	115	-102.2	11.2
PILFOG	85	-83.3	1.9
PUGPIQ	95.6	-90.1	5.7
RAFFIO01	82	-86.1	-5
SESHED	98	-98.7	-0.7
TCBZFU	125	-129.7	-3.7
TCYQME03	123.3	-116.3	5.6
THIANT03	101.1	-96.6	4.5
TOXANT	101	-93.2	7.8
ZZZAOS02	95.1	-83.8	11.9
ZZZMKS01	86	-87.4	-1.6
NAPHAC02	118.9	-111.4	6.3
ANTCEN14	97.1	-105	-8.1
ANTQUO08	111	-98	11.7
DCLANT10	114.9	-127.3	-10.7
PHENAN08	92	-97.2	-5.6
QQQFDS02	103.1	-108.4	-5.2
SAZQIT	102	-97.2	4.7
ACETAC03	64.9	-60	7.4
FORMAM02	72.1	-71.9	0.2
IMAZOL13	83.1	-88	-5.9
PYRAZI01	56.1	-62.5	-11.4
SALMID02	101	-105.3	-4.3
EJAYET	85	-78.4	7.8
ODOFO	70.9	-65.9	7.1
ZZZFHE01	66	-57.5	13
ZZZPRO08	67	-62.7	6.4