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Supplementary Information for

Revised Values for the X23 Benchmark Set of Molecular Crystals

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1 Experimental Reference Data

Table S1: Experimental data used for the back-correction of unit-cell volumes (low temperature) and sublimation enthalpies (high temperature). T_l and T_h^{exp} are the temperatures of the respective crystallographic measurements in K and V_l^{exp} and V_h^{exp} refer to the experimentally determined unit cell volumes (except stated otherwise) in Å^3. The column ”T range” lists for which temperature interval (in K) experimental heat capacities are available and T_h^{calc} refers to the temperatures used for the calculation of sublimation enthalpies (in K).

	Low Temperature				High Temperature				Exp. C_p		
System	CSD code	T_l	V_l^{exp}	Ref.	CSD code	T_h^{exp}	V_h^{exp}	Ref.	T range	Ref.	T_h^{calc}
1,4-Cyclohexanedione	CYHEXO	133	279.6	1	CYHEXO01	295	290.1	2	90-298[a]	3	298
Acetic acid	ACETAC07	40	297.3	4	ACETAC01	278	314.1	5	10-290	6	290
Adamantane	ADAMAN08	188	393.1	7	n/a	298	414.8[b]	n/a	5-298	8	298
Ammonia	n/a	2	128.6	9	n/a	171	135.6	10	2-160[a]	11	195
Anthracene	ANTCEN16	16	455.2	12	ANTCEN14	295	473.2	13	5-298	14	298
Benzene	BENZEN14	4	461.8	15	BENZEN02	270	506.6	16	4-273[a]	17,18	279
Carbon dioxide	n/a	6	171.3	19	n/a	205	187.4	19	15-190[c]	20	207
Cyanamide	CYANAM01	108	415.7	21	n/a	298	428.6[b]	n/a	90-298[a]	3	298
Cytosine	CYTSIN01	295	472.4	22	CYTSIN01	295	472.4	22	230-298[a]	23	298
Ethyl carbamate	ECARBM01	168	248.8	24	ECARBM10	295	257.7	24	90-298[a]	3	298
Formamide	FORMAM02	90	224.1	25	n/a	276	241.5[b]	n/a	90-270[a]	3	276
Hexamine	HXMTAM10	15	332.4	26	HXMTAM08	295	347.1	27	5-298	8	298
Imidazole	IMAZOL04	123	348.8	28	IMAZOL01	295	348.8	29	90-298[a]	3	298
Naphthalene	NAPHTA23	10	340.8	30	NAPHTA	295	359.3	31	10-298	32	298
Oxalic acid α	OXALAC03	295	312.6	33	OXALAC03	295	312.6	33	5-298	34	298
Oxalic acid β	OXALAC04	295	156.9	33	OXALAC04	295	156.9	33	n/a[a]	n/a	298
Pyrazine	PYRAZI01	184	203.6	35	PYRAZI	295	210.1	36	5-298	37	298
Pyrazole	PYRZOL05	108	698.3	38	PYRZOL	295	745.6	39	n/a[a]	n/a	298
s-Triazine	TRIZIN	295	586.8	40	TRIZIN	295	586.8	40	10-298	41	298
s-Trioxane	TROXAN11	103	616.5	42	TROXAN	295	638.3	43	10-298	41	298
Succinic acid	SUCACB03	77	239.3	44	SUCACB12	298	249.8	45	5-298	46	298
Uracil	URACIL	295	463.4	47	URACIL	295	463.4	47	2-298	48	298
Urea	UREAXX12	12	145.1	49	UREAXX	295	151.2	50	10-298	51	298

[a] Quasi-harmonic C_p values (PBE+D3) were used for the missing temperature range.

[b] Estimated cell volume according to eq. 5 in the main text.

[c] C_p was approximated by harmonic $C_V + R$ (PBE+D3) for the missing temperature range.

2 Thermal Pressures

Table S2: Calculated vibrational free energies (F_{vib}) for isotropically scaled unit cells and obtained thermal pressures (p_{th}) at the PBE+D3 level. The fully relaxed unit cell volumes (V_{el}) are given in Å^3 and T_l denotes the temperature in K. The superscipts in F_{vib} indicate the used scaling factor of V_{el}. The superscripts b and c in p_{th} indicate backward and central finite differences, respectively, and the number in parenthesis indicates the corresponding (scaled) unit cell volume. The step size for the finite differences is always 5 % of V_{el}. $p_{\mathrm{th}}^{\mathrm{c}}(0.95)$ and $p_{\mathrm{th}}^{\mathrm{b}}(1.0)$ are derived from the volumes with scaling factors of 0.90, 0.95, and 1.0, while $p_{\mathrm{th}}^{\mathrm{c}}(1.0)$ is calculated using the volumes with scaling factors of 0.95 and 1.05. All vibrational free energies are given in kJ/mol (per unit cell) and all thermal pressures are given in GPa. The label n/d stands for not determined.

System	T_l	V_{el}	$F_{\mathrm{vib}}^{0.90}$	$F_{\mathrm{vib}}^{0.95}$	$F_{\mathrm{vib}}^{1.0}$	$F_{\mathrm{vib}}^{1.05}$	$F_{\mathrm{vib}}^{1.10}$	$p_{\mathrm{th}}^{\mathrm{c}}(0.95)$	$p_{\mathrm{th}}^{\mathrm{c}}(1.0)$	$p_{\mathrm{th}}^{\mathrm{b}}(1.0)$
1,4-Cyclohexanedione	133	276.1	674.7	670.2	666.3	662.9	n/d	0.502	0.439	0.422
Acetic acid	40	297.6	648.8	646.4	644.5	642.8	n/d	0.242	0.197	0.181
Adamantane	188	377.8	1239.9	1232.4	1226.0	1220.2	n/d	0.614	0.536	0.523
Ammonia	2	122.6	392.9	391.7	389.9	388.7	n/d	0.414	0.402	0.567
Anthracene	16	449.9	1009.4	1004.5	1000.8	998.1	n/d	0.316	0.235	0.223
Benzene	4	457.0	1050.3	1045.8	1042.3	1039.4	n/d	0.291	0.235	0.219
Carbon dioxide	6	186.4	130.7	129.3	128.1	127.2	n/d	0.233	0.190	0.206
Cyanamide	108	413.6	726.9	725.4	723.6	721.7	n/d	0.131	0.151	0.160
Cytosine	295	466.5	977.7	969.9	963.0	956.3	n/d	0.524	0.487	0.467
Ethyl carbamate	168	241.8	552.4	548.7	545.4	542.7	n/d	0.484	0.412	0.424
Formamide	90	222.8	497.6	495.0	492.6	490.7	n/d	0.367	0.324	0.341
Hexamine	15	333.8	1022.8	1018.0	1014.6	1011.8	n/d	0.405	0.310	0.273
Imidazole	123	345.9	736.8	733.9	731.7	729.9	n/d	0.245	0.191	0.186
Naphthalene	10	337.8	767.9	764.3	761.6	759.5	n/d	0.307	0.236	0.222
Oxalic acid α	295	314.5	462.5	456.1	449.9	444.2	n/d	0.662	0.628	0.647
Oxalic acid β	295	158.7	225.0	224.4	223.6	221.7	n/d	0.150	0.285	0.194
Pyrazine	184	196.4	392.1	389.2	386.5	383.6	n/d	0.471	0.472	0.433
Pyrazole	108	704.2	1486.0	1478.9	1472.9	1467.5	1463.2	0.309	0.268	0.256
s-Triazine	295	556.5	923.5	908.5	896.1	883.7	873.9	0.817	0.740	0.662
s-Trioxane	103	615.7	1538.9	1529.0	1520.5	1513.2	n/d	0.497	0.426	0.420
Succinic acid	77	244.9	549.0	547.2	545.9	544.5	n/d	0.213	0.184	0.159
Uracil	295	457.4	847.8	841.6	836.0	830.9	n/d	0.429	0.388	0.390
Urea	12	143.8	340.8	338.8	337.1	335.6	n/d	0.426	0.374	0.372

For pyrazole and s-triazine we have calculated the following additional thermal pressures:

- at V_{el} using forward finite differences (scaling factors of 0.9, 0.95, and 1.0):
  0.280 GPa (pyrazole), 0.819 GPa (s-triazine)
- at V_{el} using central finite differences (all five data points from 0.9 to 1.1):
  0.268GPa (pyrazole), 0.740 GPa (s-triazine)
- at $1.05 \times V_{\mathrm{el}}$ using central finite differences (scaling factors of 1.0 and 1.1):
  0.229 GPa (pyrazole), 0.661 GPa (s-triazine)

Table S3: Derived thermal pressures at temperatures T_l for standard supercells ($p_{\text{th}}^{\text{std}}$) and extended supercells ($p_{\text{th}}^{\text{ext}}$) calculated with PBE+D3 for selected structures.

System	T_l / K	Standard supercell	$p_{\text{th}}^{\text{std}}$ / GPa	Extended supercell	$p_{\text{th}}^{\text{ext}}$ / GPa
1,4-Cyclohexanedione	133	$2\times2\times2$	0.439	$3\times3\times3$	0.441
Acetic acid	40	$1\times4\times3$	0.197	$2\times4\times3$	0.198
Adamantane	188	$2\times2\times2$	0.536	$3\times3\times2$	0.531
Cyanamide	108	$2\times2\times2$	0.151	$3\times3\times2$	0.150
Cytosine	295	$1\times2\times4$	0.487	$3\times2\times4$	0.522
Ethyl carbamate	168	$3\times2\times2$	0.412	$3\times3\times2$	0.412
Formamide	90	$4\times2\times2$	0.324	$5\times2\times3$	0.327
Hexamine	15	$2\times2\times2$	0.310	$3\times3\times3$	0.297
Oxalic acid α	295	$2\times2\times2$	0.628	$3\times2\times3$	0.622
Oxalic acid β	295	$3\times2\times3$	0.285	$3\times3\times3$	0.274
Pyrazine	184	$2\times3\times4$	0.472	$2\times3\times5$	0.479
Pyrazole	108	$2\times1\times2$	0.268	$2\times2\times3$	0.268
s-Triazine	295	$2\times2\times2$	0.740	$3\times3\times3$	0.703
Uracil	295	$1\times1\times4$	0.388	$2\times2\times4$	0.427

3 Thermal Expansion

Table S4: Relative volumetric expansion in % for our three DFT+D methods at a temperature T_l in K compared to fully relaxed structures at the minumum of the electronic energy. These values are compared with two force-field values and other available quantum-mechanical results from literature. Temperature differences between T_l and literature values are listed if they exceed 4 K.

System	T_l	PBE+D3	BLYP+D3	RPBE+D3	FIT[52,53]	W99rev6311P5[52,53]	others
1,4-Cyclohexanedione	133	5.7	5.4	7.5	2.4	3	
Acetic acid	40	2.3	2.5	3.6	1.6	2.3	2.2[f]
Adamantane	188	8.3	7.9	12.0	3.6	5.7	
Ammonia	2	5.4	4.8	7.0	5.8[a]	16.9[a]	3.3[g]
Anthracene	16	2.6	2.9	4.1	1.4[b]	1.8[b]	
Benzene	4	3.0	3.2	5.5	2.4[c]	10.0[c]	
Carbon dioxide	6	3.0	3.0	4.4	n/a	n/a	2.9[h]
Cyanamide	108	1.5	2.1	2.1	-2.6	4.7	
Cytosine	295	6.0	4.8	9.9	2	4.3	
Ethyl carbamate	168	6.5	6.2	9.1	2.7	3.9	
Formamide	90	4.6	4.4	7.4	2.8	3.6	
Hexamine	15	2.8	3.3	3.7	1.8[d]	1.9[d]	
Imidazole	123	3.1	3.4	4.3	2.7	3.6	3.2[f]
Naphthalene	10	2.9	3.1	4.1	1.4	1.7	
Oxalic acid α	295	5.5	5.0	7.8	5.2	6.5	
Oxalic acid β	295	2.8	4.4	4.8	5.9	9.1	
Pyrazine	184	6.6	5.5	9.5	4.5	5.6	
Pyrazole	108	4.6	4.1	6.7	7.2	9	
s-Triazine	295	12.9	8.7	(26.9)	11	11.2	
s-Trioxane	103	5.4	4.8	7.1	2.5	2.8	
Succinic acid	77	1.8	2.9	2.6	2.0[e]	3.2[e]	
Uracil	295	4.0	3.5	6.5	4.3	5.1	
Urea	12	2.4	2.9	3.5	n/a	n/a	2.6[i]

[a] $T = 160$ K; [b] $T = 94$ K; [c] $T = 218$ K; [d] $T = 120$ K; [e] $T = 298$ K; [f] MP2/aTZ result from Ref. 54; [g] PBE+MBD result for ND_3 from Ref. 55; [h] CCSD(T) result from Ref. 54; [i] DFT+D zero-point energy effects described in Ref. 56.

4 Geometries

Table S5: Unit-cell volumes (in Å^3) obtained for full lattice relaxations (V_{el}) and via the quasi-harmonic approximation (V^{QHA}) corresponding to temperatures T_l and T_h^{calc} (in K).

			PBE+D3			BLYP+D3		RPBE+D3	
System	T_l	T_h^{calc}	V_{el}	V_l^{QHA}	V_h^{QHA}	V_{el}	V_l^{QHA}	V_{el}	V_l^{QHA}
1,4-Cyclohexanedione	133	298	276.1	291.8	313.2	267.1	281.4	282.9	304.3
Acetic acid	40	290	297.6	304.4	329.7	290.4	297.7	311.1	322.3
Adamantane	188	298	377.8	409.3	431.0	365.0	393.9	385.7	431.8
Ammonia	2	195	122.6	129.2	134.3	123.0	128.9	127.1	135.9
Anthracene	16	298	449.9	461.6	488.3	429.4	441.9	441.3	459.3
Benzene	4	279	457.0	470.8	537.2	435.1	449.0	449.0	473.5
Carbon dioxide	6	207	186.4	191.9	232.7	175.8	181.1	197.3	205.9
Cyanamide	108	298	413.6	420.0	432.9	400.5	408.8	418.5	427.2
Cytosine	295	298	466.5	494.5	496.4	449.3	471.1	470.0	516.4
Ethyl carbamate	168	298	241.8	257.6	270.1	234.3	248.9	248.2	270.7
Formamide	90	276	222.8	233.0	250.4	214.1	223.6	229.7	246.6
Hexamine	15	298	333.8	343.0	367.9	325.1	335.9	335.9	348.3
Imidazole	123	298	345.9	356.7	374.4	330.2	341.4	354.4	369.6
Naphthalene	10	298	337.8	347.6	377.3	322.3	332.2	331.7	345.4
Oxalic acid α	295	298	314.5	331.8	332.4	309.0	324.4	325.3	350.8
Oxalic acid β	295	298	158.7	163.2	163.2	153.8	160.5	165.3	173.2
Pyrazine	184	298	196.4	209.4	219.4	186.6	196.9	198.0	216.8
Pyrazole	108	298	704.2	736.5	807.5	676.4	704.4	707.8	754.9
s-Triazine	295	298	556.5	628.1	629.2	528.8	574.9	567.7	720.5
s-Trioxane	103	298	615.7	649.0	704.4	594.8	623.5	640.7	686.1
Succinic acid	77	298	244.9	249.4	260.6	236.7	243.6	254.2	260.9
Uracil	295	298	457.4	475.8	476.3	440.9	456.4	464.2	494.5
Urea	12	298	143.8	147.3	154.2	142.8	147.0	146.9	152.0

Table S6: Lattice parameters for PBE+D3 optimized structures at volumes V_{el} and V_l^{QHA}. The cell lengths a, b, and c are given in Å while the cell angles α, β, and γ are given in degrees.

	PBE+D3@V_{el}						PBE+D3@V_l^{QHA}					
System	a	b	c	α	β	γ	a	b	c	α	β	γ
1,4-Cyclohexanedione	6.60	6.26	6.77	90.0	99.2	90.0	6.76	6.41	6.83	90.0	99.5	90.0
Acetic acid	13.07	3.94	5.78	90.0	90.0	90.0	13.17	3.99	5.79	90.0	90.0	90.0
Adamantane	6.55	6.55	8.80	90.0	90.0	90.0	6.73	6.73	9.05	90.0	90.0	90.0
Ammonia	4.97	4.97	4.97	90.0	90.0	90.0	5.06	5.06	5.06	90.0	90.0	90.0
Anthracene	8.39	5.95	11.09	90.0	125.6	90.0	8.49	5.98	11.14	90.0	125.3	90.0
Benzene	7.29	9.34	6.71	90.0	90.0	90.0	7.36	9.43	6.78	90.0	90.0	90.0
Carbon dioxide	5.71	5.71	5.71	90.0	90.0	90.0	5.77	5.77	5.77	90.0	90.0	90.0
Cyanamide	6.88	6.80	8.84	90.0	90.0	90.0	6.90	6.91	8.80	90.0	90.0	90.0
Cytosine	12.82	9.48	3.84	90.0	90.0	90.0	12.63	9.51	4.12	90.0	90.0	90.0
Ethyl carbamate	5.04	6.95	7.50	101.2	106.8	75.9	5.11	7.06	7.81	102.4	107.0	75.4
Formamide	3.62	8.97	6.97	90.0	100.1	90.0	3.72	9.02	7.01	90.0	98.6	90.0
Hexamine	6.94	6.94	6.94	90.0	90.0	90.0	7.00	7.00	7.00	90.0	90.0	90.0
Imidazole	7.51	5.34	9.73	90.0	117.6	90.0	7.56	5.38	9.75	90.0	116.0	90.0
Naphthalene	8.06	5.90	8.62	90.0	124.5	90.0	8.16	5.94	8.66	90.0	124.1	90.0
Oxalic acid α	6.69	7.61	6.18	90.0	90.0	90.0	6.91	7.64	6.28	90.0	90.0	90.0
Oxalic acid β	5.27	6.11	5.44	90.0	115.0	90.0	5.27	6.20	5.50	90.0	114.8	90.0
Pyrazine	9.24	5.73	3.71	90.0	90.0	90.0	9.29	5.83	3.87	90.0	90.0	90.0
Pyrazole	8.16	12.60	6.85	90.0	90.0	90.0	8.23	12.80	6.99	90.0	90.0	90.0
s-Triazine	9.58	9.58	7.00	90.0	90.0	120.0	9.80	9.80	7.55	90.0	90.0	120.0
s-Trioxane	9.36	9.36	8.12	90.0	90.0	120.0	9.51	9.51	8.28	90.0	90.0	120.0
Succinic acid	5.52	8.74	5.08	90.0	91.2	90.0	5.56	8.76	5.12	90.0	90.4	90.0
Uracil	11.94	12.24	3.67	90.0	121.6	90.0	12.01	12.27	3.76	90.0	120.9	90.0
Urea	5.55	5.55	4.67	90.0	90.0	90.0	5.61	5.61	4.68	90.0	90.0	90.0

5 Vibrational Energies

Table S7: Vibrational contributions $\Delta E_{\text{vib}}^{\text{avg}} + 4RT$ (in kJ/mol) calculated at 298 K for all systems with $T_h^{\text{calc}} < 298$ K.

System	Ref. 57	PBE+D3	BLYP+D3	RPBE+D3
Acetic acid	-4.9	-4.3	-5.4	-5.0
Ammonia	-7.4	-6.8	-7.4	-7.3
Benzene	-6.6	-5.4	-7.0	-6.0
Carbon dioxide	-3.8	-3.8	-4.0	-3.9
Formamide	-7.4	-7.0	-8.0	-7.5

Table S8: Anharmonic terms in kJ/mol corresponding to temperatures T_h^{calc} (cf. Table S1 or S5).

System	$\Delta\Delta E_{\text{latt}}^{\text{QHA}}$	$\Delta\Delta E_{\text{vib}}^{\text{QHA}}$	$\Delta\Delta E_{\text{sub}}^{\text{QHA}}$	$\Delta\Delta E_{\text{latt}}^{\text{exp}}$	$\Delta\Delta E_{\text{vib}}^{\text{exp}}$	$\Delta\Delta E_{\text{sub}}^{\text{exp}}$
1,4-Cyclohexanedione	-4.3	1.2	-3.1	-0.6	-1.4	-2.0
Acetic acid	-1.5	0.3	-1.2	-0.4	-0.7	-1.1
Adamantane	-5.6	2.1	-3.5	-2.9	-0.5	-3.4
Ammonia	-0.4	0.3	-0.1	-0.5	-0.3	-0.8
Anthracene	-3.2	1.4	-1.8	-1.2	0.2	-1.0
Benzene	-4.7	1.0	-3.7	-2.1	-1.9	-4.0
Carbon dioxide	-3.0	0.2	-2.8	0.0	-0.5	-0.5
Cyanamide	-0.2	0.1	-0.1	-0.1	-1.8	-1.9
Cytosine	-1.0	0.4	-0.6	0.0	-0.9	-0.9
Ethyl carbamate	-2.5	1.1	-1.4	-0.8	-1.8	-2.6
Formamide	-1.3	0.4	-0.9	-0.6	-1.5	-2.1
Hexamine	-3.9	1.7	-2.2	-0.6	1.1	0.5
Imidazole	-0.7	0.2	-0.5	-2.1	-1.3	-3.4
Naphthalene	-3.9	1.2	-2.7	-1.3	-0.4	-1.7
Oxalic acid α	-0.8	0.0	-0.8	0.0	-1.6	-1.6
Oxalic acid β	-0.2	0.1	-0.1	-0.1	-0.3	-0.4
Pyrazine	-2.4	0.5	-1.9	-0.9	-0.8	-1.7
Pyrazole	-2.3	0.6	-1.7	-0.4	-0.6	-1.0
s-Triazine	-3.0	0.3	-2.7	-0.6	-0.5	-1.1
s-Trioxane	-3.7	1.6	-2.1	-0.2	-0.6	-0.8
Succinic acid	-1.1	0.3	-0.8	-0.1	-2.7	-2.8
Uracil	-0.4	0.2	-0.2	0.0	-0.7	-0.7
Urea	-1.3	0.4	-0.9	-0.7	-0.4	-1.1

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