Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Cohesive Properties of the Crystalline Phases of Twenty Proteinogenic α-Aminoacids from First-principles calculations

Supporting Information

Ctirad Červinka,[†,*] *Michal Fulem*

[†] Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, CZ-166 28 Prague 6, Czech Republic

*Corresponding author: cervinkc@vscht.cz

TABLE S1

Cohesive energies (E_{coh}, kJ·mol^{-1}) calculated using various computational setups (500 or 900 eV plane-wave energy cutoff values and PBE or PBEsol functionals, both used with the D3(BJ) correction). Data set used in this work for calculation of the sublimation enthalpies exploiting the CCSD(T)-F12 refinements of the proton transfer energies are given for comparison.

Functional	PBE_{900}	PBE_{500}	$PBEsol_{900}$	$PBEsol_{500}$	PBE_{900}+CCSD(T)-F12
Amino acid			$-E_{coh}$		
Alanine	153.6	157.4	159.2	163.0	135.4
Serine	159.2	163.7	182.1	184.9	145.8
Tyrosine	205.3	210.4	227.3	232.2	195.1

TABLE S2

Experimental unit-cell parameters (in Å, degrees, first row for each amino acid) compared to their optimized (with respect to the electronic energy only) counterparts obtained using either periodic PBE-D3(BJ) calculations in VASP (second row for each amino acid) or Amoeba-based calculations in Tinker (third row for each amino acid). Structures were optimized with respect to their static electronic energy only.

Amino acid	***a***	***b***	***c***	***α***	***β***	***γ***	Ref.
Glycine	6.7390	6.7390	5.3640	90.00	90.00	120.00	[1]
	7.0855	7.0855	5.5039	90.00	90.00	120.00	
	7.0063	7.0065	5.7480	90.00	90.00	120.00	
Alanine	6.0190	12.3300	5.7830	90.00	90.00	90.00	[2]
	6.0841	12.1071	5.8455	90.00	90.00	90.00	
	5.5422	13.3511	5.8159	90.00	90.00	90.00	
Valine	9.6820	5.2470	11.9300	90.00	90.57	90.00	[3]
	9.6738	5.2347	11.9081	90.00	90.72	90.00	
	10.0508	5.1802	11.8410	90.00	91.74	90.00	
Leucine	9.5620	5.3010	14.5190	90.00	94.20	90.00	[4]
	9.6033	5.2779	14.5516	90.00	94.74	90.00	
	10.0856	5.2234	14.4913	90.00	96.74	90.00	
Isoleucine	9.6810	5.3010	13.9560	90.00	96.16	90.00	[5]
	9.6744	5.2698	13.9700	90.00	95.50	90.00	
	10.1959	5.1148	13.7628	90.00	93.46	90.00	

Serine	5.5900	8.5690	9.2330	90.00	90.00	90.00	6
	5.6432	8.4961	9.4469	90.00	90.00	90.00	
	5.6775	8.6001	9.3578	90.00	90.00	90.00	
Threonine	13.6280	7.6180	5.1100	90.00	90.00	90.00	7
	13.6050	7.8011	5.1202	90.00	90.00	90.00	
	14.2849	7.3131	5.1769	90.00	90.00	90.00	
Cysteine	8.1430	11.9370	5.4160	90.00	90.00	90.00	8
	8.0878	11.8962	5.4210	90.00	90.00	90.00	
	9.0230	11.7727	5.7292	90.00	90.00	90.00	
Methionine	9.4930	5.2010	14.8310	90.00	99.84	90.00	3
	9.5385	5.2071	14.7886	90.00	100.25	90.00	
	10.0521	5.1398	14.4721	90.00	99.87	90.00	
Aspartic acid	5.1140	6.9060	7.5930	90.00	100.66	90.00	9
	5.1467	6.9813	7.6386	90.00	99.12	90.00	
	5.0736	6.8763	7.8709	90.00	102.08	90.00	
Asparagine	5.0620	6.7000	8.0540	90.00	91.71	90.00	10
	5.0953	6.8110	8.0683	90.00	90.96	90.00	
	5.0286	7.0476	8.1197	90.00	96.83	90.00	
Glutamic acid	10.2820	8.7790	7.0680	90.00	90.00	90.00	11
	10.2787	8.7590	7.1567	90.00	90.00	90.00	
	10.2770	8.5950	7.5213	90.00	90.00	90.00	
Glutamine	15.4500	7.5500	4.9720	90.00	90.00	90.00	12
	15.9533	7.8112	5.0894	90.00	90.00	90.00	
	16.6812	7.8645	5.1091	90.00	90.00	90.00	
Arginine	9.7570	16.0230	5.5800	90.00	98.06	90.00	13
	9.6819	16.0585	5.5547	90.00	94.47	90.00	
	9.6877	16.9640	5.4395	90.00	89.96	90.00	
Lysine	9.5060	5.1290	16.9940	90.00	97.70	90.00	14
	9.4734	5.0911	17.3102	90.00	94.99	90.00	
	9.9881	5.0373	16.2179	90.00	95.97	90.00	
Histidine	5.1770	7.3220	18.8700	90.00	90.00	90.00	15
	5.1549	7.3353	18.8487	90.00	90.00	90.00	
	5.1300	7.3089	18.9250	90.00	90.00	90.00	
Proline	11.5500	9.0200	5.2000	90.00	90.00	90.00	16
	11.6826	8.8979	5.2989	90.00	90.00	90.00	
	11.5100	8.7088	5.7150	90.00	90.00	90.00	
Phenylalanine	8.7830	5.9980	31.0180	90.00	96.95	90.00	17
	8.8143	6.0504	31.1018	90.00	97.21	90.00	
	9.0011	6.0344	30.8626	90.00	97.70	90.00	

Tyrosine	6.9130	21.1180	5.8320	90.00	90.00	90.00	[18]
	6.7035	21.1085	5.8412	90.00	90.00	90.00	
	6.4880	22.2104	5.9569	90.00	90.00	90.00	
Tryptophan	11.4300	11.4640	35.6060	84.42	87.69	60.10	[19]
	11.3574	11.5099	35.8149	84.31	87.70	60.46	
	11.5756	11.2777	35.6299	84.55	87.29	59.23	

TABLE S3

Comparison of the proton transfer energies $\Delta_{PT}E$ (kJ mol^{-1}) calculated at the CCSD(T)-F12/aug-cc-pVDZ level of theory. The underlying molecular geometries were previously optimized at the PBE-D3(BJ) level of theory, using the projector-augmented wave (PAW) method for the zwitterion and the PAW or the Gaussian atomic basis set 6-311+G(d,p).

Amino acid	$\Delta_{PT}E_{G}^{PAW}$	$\Delta_{PT}E_{PAW}^{PAW}$	Amino acid	$\Delta_{PT}E_{G}^{PAW}$	$\Delta_{PT}E_{PAW}^{PAW}$
Glycine	142.32	144.98	Asparagine	154.90	156.36
Alanine	137.80	138.67	Glutamic acid	180.35	181.66
Valine	132.40	134.84	Glutamine	145.32	145.57
Leucine	132.21	134.88	Arginine	219.01	221.61
Isoleucine	132.12	133.59	Lysine	136.89	138.45
Serine	160.34	161.93	Histidine	99.96	101.39
Threonine	112.70	113.95	Proline	109.54	110.53
Cysteine	149.09	150.53	Phenylalanine	147.53	148.77
Methionine	133.04	135.05	Tyrosine	142.89	144.22
Aspartic acid	168.37	169.56	Tryptophan	148.82	152.60

TABLE S4

Comparison of the difference of the zero point vibrational energies of the vapor and crystalline phases ($\Delta_{ZPE}E$, kJ·mol^{-1}) calculated using various computational setups (500 or 900 eV plane-wave energy cutoff values and PBE or PBEsol functionals, both used with the D3(BJ) correction).

Functional	PBE_{900}	PBE_{500}	$PBEsol_{900}$	$PBEsol_{500}$
Amino acid		$-\Delta_{ZPE}E$		
Alanine	10.89	10.13	8.81	8.73
Serine	8.08	7.18	8.56	8.91
Tyrosine	10.50	10.32	9.98	9.86

TABLE S5

Experimental isobaric heat capacities ($C_p^{cr,exp}$, J K^{-1} mol^{-1}) at 300 K along with the values calculated using the simplifying scheme A3 ($C_p^{cr,A3}$**)** and their relative percentage deviations from the experimental value (δ_C) .

Amino acid	$C_p^{cr,A3}$	$C_p^{cr,exp}$	δ_C	Ref.	Amino acid	$C_p^{cr,A3}$	$C_p^{cr,exp}$	δ_C	Ref.
Glycine	91.5	96.4	−5.1%	[20]	Asparagine	155.1	161.2	−3.8%	[21]
Alanine	116.4	122.8	−5.2%	[22]	Glutamic acid	168.8	176.1	−4.2%	[21]
Valine	163.5	169.6	−3.2%	[23]	Glutamine	179.4	185.1	−3.1%	[24]
Leucine	180.2	202.5	−11.0%	[23]	Arginine	222.6	234.5	−5.1%	[25]
Isoleucine	183.0	189.3	−3.3%	[23]	Lysine	-	-	-	-
Serine	130.6	136.0	−4.0%	[26]	Histidine	-	-	-	-
Threonine	152.9	-	-	-	Proline	139.3	152.1	−8.4%	[27]
Cysteine	142.0	160.3	−11.4%	[28]	Phenylalanine	192.0	204.2	−6.0%	[27]
Methionine	184.8	205.1	−9.9%	[29]	Tyrosine	208.8	218.4	−4.4%	[25]
Aspartic acid	149.2	155.1	−3.9%	[21]	Tryptophan	-	239.6	-	[27]

TABLE S6

Sublimation enthalpies at 298.15 K ($\Delta_{sub}H(298.15\ K)$ in kJ mol^{-1}), calculated in this work by A3 approximation along with those derived from critically assessed enthalpies of formation reported by Dorofeeva and Ryzhova [30] and absolute deviation δ_H in kJ mol^{-1}.

	$\Delta_{sub}H(298.15\ K)$	$\Delta_{sub}H(298.15\ K)$	δ_H
	This work, A3	Dorofeeva and Ryzhova. [30]	
Glycine	134.7	134.4	0.3
Alanine	124.4	135.2	-10.8
Valine	126.5	138.9	-12.4
Leucine	130.7	139.8	-9.1
Isoleucine	131.3	141.4	-10.1
Serine	132.4	146.8	-14.4
Threonine	140.7	165.4	-24.7
Cysteine	128.8	133.7	-4.9
Methionine	141.8	147.7	-5.9
Aspartic acid	165.6	176.5	-10.9
Asparagine	161.5	174.2	-12.7
Glutamic acid	176.5	190.3	-13.8
Glutamine	171.1	194.8	-23.7
Arginine	202.1	210.4	-8.3
Lysine	150.1	213.7	-63.6
Histidine	165.2	177.3	-12.1
Proline	111.8	125.7	-13.9
Phenylalanine	145.1	146.4	-1.3
Tyrosine	183.3	185.5	-2.2
Tryptophan	154.2[a]	167.7	-13.5

[a] calculated by A1 approximation

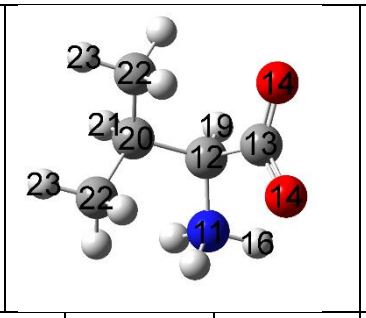
TABLE S7

Atomic multipoles parametrized for amino acid zwitterions, compatible with the standard setting of the Amoeba force field. Charge unit is the elementary charge, distance unit is Å. First row lists the definition of the coordinates of the local atomic multipole frame, defined through the common Amoeba conventions, and the partial atomic charge, second row lists the atomic dipole with respect to the local frame, last three rows contain the atomic quadrupole. Note that the numbering of the atomic types is not compatible with any of the Amoeba distributions and needs to be adjusted if necessary.

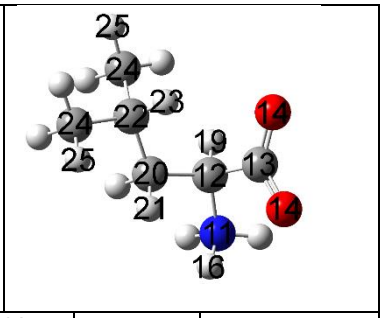
S7.1 Glycine							**S7.2 Alanine**					
11	12	16	0.36475				11	12	16	0.42682		
			0.01127	0.00000	0.32627					-0.06068	0.00000	0.45169
			-0.34967							-0.16891		
			0.00000	-0.39511						0.00000	-0.45554	
			0.09736	0.00000	0.74478					-0.12207	0.00000	0.62445
12	11	13	-0.36816				12	11	13	-0.42411		
			-0.11745	0.00000	0.49851					-0.08298	0.00000	0.30672
			-1.43557							-1.53562		
			0.00000	-0.33197						0.00000	-0.85978	
			-0.95822	0.00000	1.76754					-0.30169	0.00000	2.39540
13	-14	-14	1.05675				13	-14	-14	1.02867		
			-0.00925	0.00000	-0.13578					0.08771	0.00000	-0.27605
			-0.00352							-0.59087		
			0.00000	-0.78860						0.00000	-0.67709	
			0.11313	0.00000	0.79212					-0.64881	0.00000	1.26796
14	13	14	-0.86405				14	13	14	-0.85136		
			0.20679	0.00000	-0.08733					0.22748	0.00000	-0.07277
			-0.64496							-0.81328		
			0.00000	0.14813						0.00000	0.19174	
			0.08699	0.00000	0.49683					0.16758	0.00000	0.62154
16	11	12	0.18374				16	11	12	0.17360		
			0.03611	0.00000	-0.20486					0.03251	0.00000	-0.31897
			0.06455							0.23986		
			0.00000	0.04177						0.00000	0.08722	
			0.03154	0.00000	-0.10632					0.02248	0.00000	-0.32708
19	12	11	0.06177				19	12	11	0.06045		
			-0.07713	0.00000	0.05928					-0.18883	0.00000	0.16486
			-0.14234							-0.22637		
			0.00000	0.15592						0.00000	0.15389	
			-0.15418	0.00000	-0.01358					-0.44652	0.00000	0.07248

							20	12	21	-0.12084		
										-0.13630	0.00000	0.32276
										-0.19196		
										0.00000	-0.00216	
										-0.18492	0.00000	0.19412
							21	20	12	0.07031		
										-0.00384	0.00000	-0.03776
										0.01274		
										0.00000	-0.04843	
										0.01311	0.00000	0.03569

S7.3 Valine



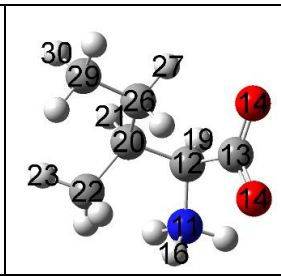
S7.4 Leucine



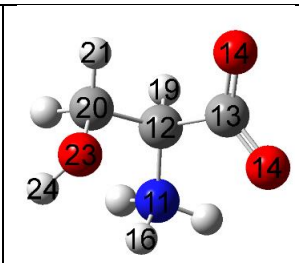
11	12	16	0.36551				11	12	16	0.36962		
			-0.03798	0.00000	0.33056					-0.13061	0.00000	0.40841
			0.20388							0.49608		
			0.00000	-0.11621						0.00000	0.16030	
			-0.07607	0.00000	-0.08767					-0.28848	0.00000	-0.65638
12	11	13	-0.31607				12	11	13	-0.31145		
			-0.25275	0.00000	0.36099					-0.16687	0.00000	0.39010
			-0.57553							-0.15715		
			0.00000	0.11868						0.00000	0.24637	
			-0.30275	0.00000	0.45685					-0.17877	0.00000	-0.08922
13	-14	-14	1.11904				13	-14	-14	1.08813		
			0.15720	0.00000	-0.18414					0.17238	0.00000	-0.23618
			0.13811							-0.11055		
			0.00000	-0.98416						0.00000	-0.72122	
			-0.26161	0.00000	0.84605					-0.31762	0.00000	0.83177
14	13	14	-0.87674				14	13	14	-0.85971		
			0.24412	0.00000	-0.15372					0.25101	0.00000	-0.11863
			-0.65822							-0.65962		
			0.00000	0.20384						0.00000	0.15320	
			0.18479	0.00000	0.45438					0.23578	0.00000	0.50642
16	11	12	0.16299				16	11	12	0.12003		
			-0.03799	0.00000	-0.19289					-0.15520	0.00000	-0.21135
			0.06126							0.03122		
			0.00000	-0.04742						0.00000	-0.03253	
			-0.04921	0.00000	-0.01384					-0.14951	0.00000	0.00131
19	12	11	0.02782				19	12	11	0.04058		
			0.00515	0.00000	0.11681					-0.13191	0.00000	0.09113
			-0.09010							0.08126		
			0.00000	0.06569						0.00000	-0.08498	
			0.17321	0.00000	0.02441					-0.05400	0.00000	0.00372
20	12	22	-0.11283				20	12	23	-0.14493		
			-0.02630	0.00000	0.26225					0.13065	0.00000	0.21355
			-0.50829							0.12988		
			0.00000	-0.60491						0.00000	-0.33421	
			0.19819	0.00000	1.11320					0.11897	0.00000	0.20433
21	20	12	0.08408				21	20	12	0.04637		
			-0.00391	0.00000	-0.05601					0.09224	0.00000	-0.08504
			-0.15620							0.15703		

			0.00000	0.39759					0.00000	0.02604	
			0.03913	0.00000	-0.24139				0.08600	0.00000	-0.18307
22	20	23	-0.17049			23	20	25	-0.04681		
			0.00399	0.00000	0.28623				-0.03351	0.00000	0.24595
			-0.50748						-0.20125		
			0.00000	-0.53179					0.00000	-0.20978	
			0.01561	0.00000	1.03927				-0.10890	0.00000	0.41103
23	22	20	0.07299			24	23	20	0.05803		
			-0.01161	0.00000	-0.12845				-0.03606	0.00000	0.05943
			-0.08643						0.03064		
			0.00000	0.10044					0.00000	-0.08814	
			0.00022	0.00000	-0.01401				-0.04257	0.00000	0.05750
						25	23	26	-0.15486		
									0.03211	0.00000	0.21902
									-0.48123		
									0.00000	-0.50532	
									0.09777	0.00000	0.98655
						26	25	23	0.08719		
									0.05069	0.00000	-0.01898
									-0.09031		
									0.00000	-0.00286	
									0.05454	0.00000	0.09317

S7.5 Isoleucine



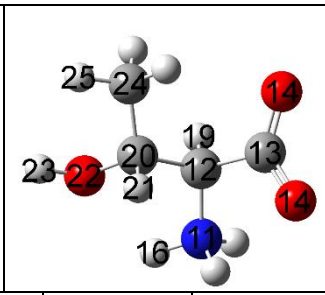
S7.6 Serine



11	12	16	0.33059				11	12	16	0.45629		
			-0.00975	0.00000	0.34509					-0.00660	0.00000	0.46885
			-0.11926							-0.09195		
			0.00000	-0.47338						0.00000	-0.55469	
			0.18216	0.00000	0.59264					0.05965	0.00000	0.64664
12	11	13	-0.32167				12	11	13	-0.51136		
			-0.26500	0.00000	0.34923					-0.29219	0.00000	0.39063
			-0.78656							-1.31895		
			0.00000	0.41551						0.00000	-0.63736	
			-0.06709	0.00000	0.37105					-0.46074	0.00000	1.95631
13	-14	-14	0.99392				13	-14	-14	1.08899		
			-0.00358	0.00000	-0.17797					0.00917	0.00000	-0.21667
			-0.00150							-0.16119		
			0.00000	-0.49572						0.00000	-0.31526	
			0.48366	0.00000	0.49722					0.42581	0.00000	0.47645
14	13	14	-0.85852				14	13	14	-0.88634		
			0.26647	0.00000	-0.14658					0.28206	0.00000	-0.16029
			-0.56430							-0.66027		
			0.00000	0.11041						0.00000	0.19632	
			0.30629	0.00000	0.45389					0.23014	0.00000	0.46395
16	11	12	0.18231				16	11	12	0.16222		
			-0.00555	0.00000	-0.22267					-0.04023	0.00000	-0.16212
			0.04965							-0.02515		
			0.00000	0.01787						0.00000	-0.00287	
			0.03349	0.00000	-0.06752					-0.04201	0.00000	0.02802
19	12	11	0.04992				19	12	11	0.06084		
			-0.02306	0.00000	0.09681					-0.03210	0.00000	0.18140

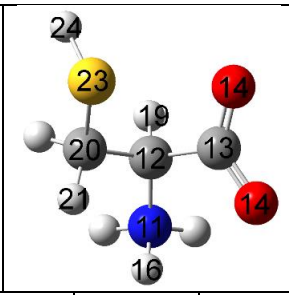
			-0.19115							-0.14374		
			0.00000	0.23020						0.00000	0.13145	
			-0.03313	0.00000	-0.03905					-0.10112	0.00000	0.01229
20	12	26	-0.04251				20	23	12	0.23170		
			0.29791	0.00000	0.25489					0.42021	0.00000	0.15858
			0.25447							-0.23995		
			0.00000	-0.19914						0.00000	-0.40268	
			-0.14486	0.00000	-0.05533					-0.31402	0.00000	0.64263
21	20	12	0.09883				21	20	23	0.06336		
			-0.02377	0.00000	-0.03530					0.06221	0.00000	-0.13386
			-0.29839							0.00249		
			0.00000	0.39898						0.00000	0.14257	
			0.07891	0.00000	-0.10059					0.06589	0.00000	-0.14506
22	20	23	-0.15833				23	20	24	-0.40572		
			0.01225	0.00000	0.36525					0.20168	0.00000	0.23830
			-0.52666							0.26442		
			0.00000	-0.21819						0.00000	-0.76960	
			-0.03704	0.00000	0.74485					-0.17914	0.00000	0.50518
23	22	20	0.10165				24	23	20	0.23856		
			-0.03005	0.00000	-0.05297					-0.04242	0.00000	-0.00895
			-0.12874							-0.09512		
			0.00000	0.08794						0.00000	-0.15774	
			-0.08618	0.00000	0.04080					0.04303	0.00000	0.25286
26	20	29	-0.14436									
			0.06136	0.00000	0.20926							
			-0.94711									
			0.00000	0.10287								
			-1.03696	0.00000	0.84424							
27	26	20	0.06926									
			0.00496	0.00000	-0.12648							
			-0.08619									
			0.00000	0.39252								
			0.21812	0.00000	-0.30633							
29	26	30	-0.17995									
			0.07172	0.00000	0.28590							
			0.14897									
			0.00000	-1.09093								
			-0.31645	0.00000	0.94196							
30	29	26	0.03340									
			-0.07434	0.00000	-0.23422							
			-0.00723									
			0.00000	0.01678								
			-0.02810	0.00000	-0.00955							

S7.7 Threonine

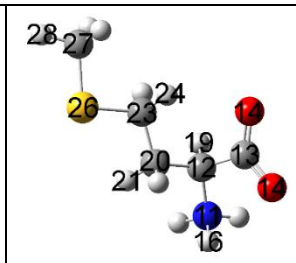
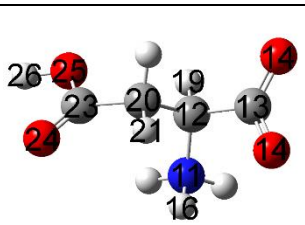


11	12	16	0.37702				11	12	16	0.42899		
			-0.15773	0.00000	0.44066					0.01266	0.00000	0.74358
			-1.52603							-0.00677		
			0.00000	-1.52951						0.00000	-0.03677	
			-0.35391	0.00000	3.05554					0.06024	0.00000	0.04354
12	11	13	-0.37032				12	11	13	-0.48204		

S7.8 Cysteine

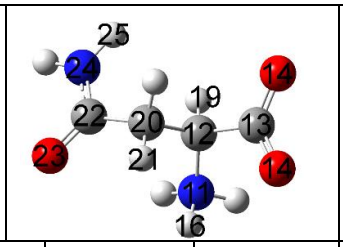


			0.05599	0.00000	0.24597					0.55169	0.00000	0.43026
			-1.03291							0.33185		
			0.00000	-1.14662						0.00000	-1.65924	
			0.20230	0.00000	2.17953					-0.91303	0.00000	1.32739
13	-14	-14	1.01064				13	-14	-14	1.08107		
			0.04767	0.00000	-0.30550					-0.11435	0.00000	-0.52332
			-0.16165							-1.01593		
			0.00000	-1.19610						0.00000	-1.74509	
			-0.29730	0.00000	1.35775					0.29851	0.00000	2.76102
14	13	14	-0.82908				14	13	14	-0.84735		
			0.15562	0.00000	0.04623					0.14012	0.00000	0.07719
			-0.81043							-0.97883		
			0.00000	0.11803						0.00000	0.21622	
			0.05186	0.00000	0.69240					0.08873	0.00000	0.76261
16	11	12	0.17588				16	11	12	0.17977		
			0.16229	0.00000	-0.41169					-0.09188	0.00000	-0.12727
			0.09422							0.03791		
			0.00000	0.32084						0.00000	-0.04594	
			0.14253	0.00000	-0.41506					-0.04580	0.00000	0.00803
19	12	11	0.07208				19	12	11	0.06231		
			-0.08941	0.00000	0.25249					-0.04870	0.00000	0.18443
			-0.08253							0.00680		
			0.00000	-0.00634						0.00000	-0.00856	
			-0.32913	0.00000	0.08887					-0.07789	0.00000	0.00176
20	22	12	0.07029				20	23	12	0.02720		
			0.11126	0.00000	0.05473					0.12491	0.00000	-0.21406
			-1.12455							-0.56020		
			0.00000	-0.30925						0.00000	-0.47059	
			0.07615	0.00000	1.43380					-0.47895	0.00000	1.03079
21	20	22	0.04119				21	20	23	0.08659		
			0.13402	0.00000	-0.01013					0.09951	0.00000	-0.06071
			-0.09247							-0.03226		
			0.00000	0.15075						0.00000	-0.01307	
			0.11723	0.00000	-0.05828					0.04880	0.00000	0.04533
22	20	23	-0.38563				23	20	24	-0.03622		
			-0.02957	0.00000	0.47548					0.32719	0.00000	0.06416
			-0.19306							1.38888		
			0.00000	-1.01212						0.00000	-2.08494	
			-0.74343	0.00000	1.20518					-0.80990	0.00000	0.69606
23	22	20	0.23025				24	23	20	-0.09910		
			0.09276	0.00000	-0.02931					0.09763	0.00000	-0.15610
			0.01523							0.00122		
			0.00000	-0.03049						0.00000	-0.07222	
			0.06478	0.00000	0.01526					0.14982	0.00000	0.07100
24	20	25	-0.13913									
			0.01461	0.00000	0.30866							
			0.05968									
			0.00000	-0.16451								
			-0.03294	0.00000	0.10483							
25	24	20	0.07471									
			-0.00804	0.00000	0.02958							
			-0.05061									
			0.00000	-0.08263								
			0.02573	0.00000	0.13324							

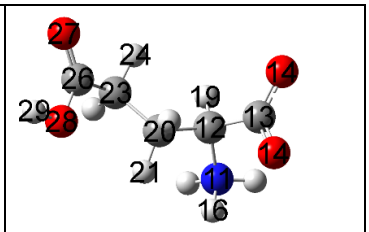
S7.9 Methionine							**S7.10 Aspartic acid**					
11	12	16	0.38015				11	12	16	0.38733		
			-0.05821	0.00000	0.41207					-0.18669	0.00000	0.36672
			0.29496							-0.51550		
			0.00000	-0.08495						0.00000	-0.98799	
			-0.06476	0.00000	-0.21001					-0.40950	0.00000	1.50349
12	11	13	-0.33917				12	11	13	-0.34399		
			-0.10999	0.00000	0.47711					0.17083	0.00000	0.23950
			-0.03442							-0.22629		
			0.00000	0.38857						0.00000	-0.36314	
			-0.36665	0.00000	-0.35415					-0.51191	0.00000	0.58943
13	-14	-14	1.13272				13	-14	-14	0.96499		
			0.20015	0.00000	-0.19286					0.03901	0.00000	-0.08419
			0.47381							-0.05579		
			0.00000	-1.49830						0.00000	-0.73203	
			-0.44405	0.00000	1.02449					-0.10086	0.00000	0.78782
14	13	14	-0.84796				14	13	14	-0.82635		
			0.25688	0.00000	0.02364					0.17612	0.00000	-0.03766
			-0.93824							-0.64131		
			0.00000	0.08951						0.00000	0.14333	
			0.24801	0.00000	0.84873					0.17323	0.00000	0.49798
16	11	12	0.08897				16	11	12	0.18125		
			-0.13245	0.00000	-0.25606					0.02688	0.00000	-0.37753
			0.00356							0.10346		
			0.00000	0.04205						0.00000	0.15421	
			-0.15355	0.00000	-0.04561					0.00839	0.00000	-0.25767
19	12	11	0.05472				19	12	11	0.07656		
			0.02477	0.00000	0.18453					-0.13262	0.00000	-0.04517
			-0.03143							0.12677		
			0.00000	-0.12575						0.00000	0.03719	
			0.17575	0.00000	0.15718					-0.24908	0.00000	-0.16396
20	23	12	-0.07865				20	23	12	-0.15151		
			0.32142	0.00000	0.12260					0.33866	0.00000	0.34431
			0.30979							-2.58654		
			0.00000	-0.73292						0.00000	1.02952	
			-0.36100	0.00000	0.42313					1.42622	0.00000	1.55702
21	20	12	0.11052				21	20	12	0.11732		
			0.04517	0.00000	-0.05816					-0.28577	0.00000	0.10208
			0.04132							0.10373		
			0.00000	0.03051						0.00000	-0.27443	
			0.04111	0.00000	-0.07183					-0.28086	0.00000	0.17070
23	26	20	-0.03673				23	24	25	0.76834		
			0.17250	0.00000	0.20469					-0.13294	0.00000	0.05447
			-0.17937							0.71253		
			0.00000	-0.16103						0.00000	-0.54273	
			-0.17284	0.00000	0.34040					-0.68929	0.00000	-0.16980
24	23	26	0.08186				24	23	25	-0.64624		
			-0.01471	0.00000	-0.02813					0.06440	0.00000	0.01538
			-0.02744							-0.66466		
			0.00000	0.03978						0.00000	0.23035	
			-0.05100	0.00000	-0.01234					0.03576	0.00000	0.43431
26	23	27	-0.25163				25	23	26	-0.43919		
			0.20930	0.00000	0.26901					0.15381	0.00000	0.01914

			1.05503							0.03743		
			0.00000	-2.46581						0.00000	-0.44366	
			-0.79568	0.00000	1.41078					-0.29989	0.00000	0.40623
27	26	28	-0.01831				26	25	23	0.25802		
			0.03442	0.00000	0.48143					0.09992	0.00000	-0.13537
			-0.78160							0.09053		
			0.00000	-0.56523						0.00000	-0.04079	
			-0.15314	0.00000	1.34683					0.15533	0.00000	-0.04974
28	27	26	0.06705									
			0.03317	0.00000	-0.12640							
			0.00115									
			0.00000	0.04624								
			0.03293	0.00000	-0.04739							

S7.11 Asparagine



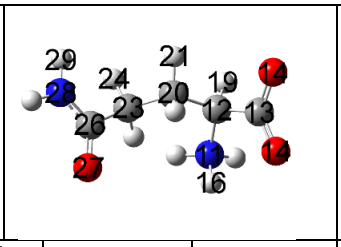
S7.12 Glutamic acid



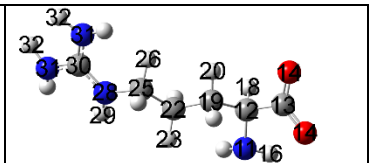
11	12	16	0.39353				11	12	16	0.30264		
			-0.03467	0.00000	0.45662					-0.00843	0.00000	0.30520
			-1.65874							-0.05092		
			0.00000	-1.62716						0.00000	-0.47566	
			-0.10908	0.00000	3.28590					-0.09394	0.00000	0.52658
12	11	13	-0.39868				12	11	13	-0.30153		
			0.32058	0.00000	0.29252					-0.24125	0.00000	0.34832
			-0.13705							-0.64396		
			0.00000	-0.66121						0.00000	-0.09661	
			-0.60273	0.00000	0.79826					-0.59162	0.00000	0.74057
13	-14	-14	0.99148				13	-14	-14	0.91275		
			0.03808	0.00000	-0.41112					0.02217	0.00000	-0.17562
			-1.17291							-0.25259		
			0.00000	-1.13753						0.00000	-0.58817	
			-0.30562	0.00000	2.31044					-0.19667	0.00000	0.84076
14	13	14	-0.83174				14	13	14	-0.80009		
			0.13736	0.00000	-0.04382					0.22472	0.00000	-0.06252
			-0.78556							-0.68003		
			0.00000	0.23825						0.00000	0.13269	
			0.12112	0.00000	0.54731					0.24350	0.00000	0.54734
16	11	12	0.18582				16	11	12	0.18175		
			0.17394	0.00000	-0.51204					0.00535	0.00000	-0.19490
			0.12177							0.02941		
			0.00000	0.42135						0.00000	0.01105	
			0.12632	0.00000	-0.54312					0.00055	0.00000	-0.04046
19	12	11	0.06274				19	12	11	0.08035		
			-0.07954	0.00000	0.06364					-0.01834	0.00000	0.04704
			0.32113							0.27154		
			0.00000	-0.08257						0.00000	0.01231	
			-0.15322	0.00000	-0.23856					0.18781	0.00000	-0.28385
20	23	12	-0.15214				20	12	23	-0.07880		
			0.53082	0.00000	0.21204					0.17781	0.00000	0.29622
			-1.60850							-0.24686		
			0.00000	-0.26418						0.00000	-0.56786	
			-0.28848	0.00000	1.87268					-0.23491	0.00000	0.81472
21	20	12	0.11080				21	20	12	0.06729		
			-0.19962	0.00000	-0.06354					-0.04280	0.00000	-0.08791

			0.11251							-0.09101			
			0.00000	0.01033						0.00000	0.12147		
			-0.16911	0.00000	-0.12284					-0.09548	0.00000	-0.03046	
23	24	25	0.71367				23	26	20	-0.21511			
			0.16422	0.00000	0.40671					0.26572	0.00000	0.14772	
			1.53142							0.09625			
			0.00000	-0.57282						0.00000	-0.66920		
			0.86410	0.00000	-0.95860					-0.28595	0.00000	0.57295	
24	23	25	-0.76369				24	23	20	0.12006			
			-0.13655	0.00000	-0.15718					0.04769	0.00000	-0.11240	
			-0.56265							0.13935			
			0.00000	0.25386						0.00000	0.00533		
			-0.05279	0.00000	0.30879					0.04373	0.00000	-0.14468	
25	23	26	-0.24149				26	28	27	0.79882			
			-0.14172	0.00000	0.00165					0.09955	0.00000	0.02089	
			0.25379							0.38934			
			0.00000	-0.98402						0.00000	-0.33071		
			-0.26238	0.00000	0.73023					-0.05427	0.00000	-0.05863	
26	25	23	0.13950				27	26	29	-0.40398			
			0.02932	0.00000	-0.16123					0.23686	0.00000	0.05463	
			0.01468							0.36704			
			0.00000	-0.00990						0.00000	-0.60578		
			0.02686	0.00000	-0.00478					-0.23727	0.00000	0.23874	
							28	26	27	-0.66519			
										-0.05778	0.00000	-0.09941	
										-0.48993			
										0.00000	0.16435		
										-0.04442	0.00000	0.32558	
							29	27	26	0.25028			
										-0.03898	0.00000	-0.08779	
										-0.02182			
										0.00000	-0.05970		
										-0.01078	0.00000	0.08152	

S7.13 Glutamine



S7.14 Arginine

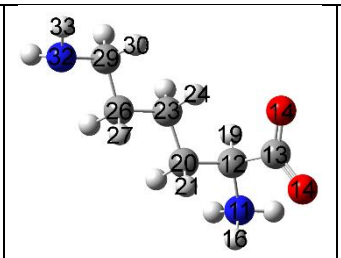


11	12	16	0.45507				11	12	16	-0.28776			
			-0.01412	0.00000	0.43326					-0.09329	0.00000	0.67350	
			-0.18632							-0.34253			
			0.00000	-0.68833						0.00000	-0.52598		
			0.09237	0.00000	0.87465					-0.33905	0.00000	0.86851	
12	11	13	-0.51278				12	11	13	-0.26786			
			0.01262	0.00000	0.45837					-0.16964	0.00000	0.12951	
			-0.37795							-0.88102			
			0.00000	-0.42355						0.00000	0.74617		
			-0.23905	0.00000	0.80150					-0.35081	0.00000	0.13485	
13	-14	-14	1.04657				13	-14	-14	1.09833			
			0.12563	0.00000	-0.28590					-0.15497	0.00000	-0.03285	
			-0.42489							0.40161			
			0.00000	-1.08391						0.00000	-0.68897		
			-0.50193	0.00000	1.50880					0.19186	0.00000	0.28736	
14	13	14	-0.84450				14	13	14	-0.87595			
			0.20049	0.00000	-0.03482					0.21381	0.00000	-0.10390	
			-0.81824							-0.55088			

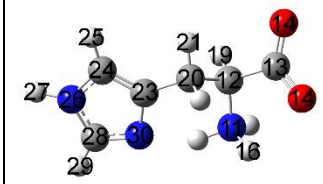
			0.00000	0.17616						0.00000	0.06124	
			0.15549	0.00000	0.64208					0.23813	0.00000	0.48964
16	11	12	0.17464				16	11	12	0.08235		
			0.01875	0.00000	-0.23902					-0.12725	0.00000	-0.42671
			0.03320							0.26415		
			0.00000	0.08950						0.00000	0.20265	
			0.02911	0.00000	-0.12270					-0.17311	0.00000	-0.46680
19	12	11	0.07722				18	12	11	-0.06375		
			-0.10914	0.00000	0.22269					-0.18275	0.00000	-0.11863
			-0.01267							0.21321		
			0.00000	-0.06554						0.00000	0.12828	
			-0.18350	0.00000	0.07821					-0.29436	0.00000	-0.34149
20	12	23	-0.04325				19	12	22	-0.11141		
			0.37379	0.00000	0.18842					0.19546	0.00000	0.14228
			0.38547							-0.09705		
			0.00000	0.24173						0.00000	-0.51284	
			-0.14306	0.00000	-0.62720					-0.22709	0.00000	0.60989
21	20	12	0.09544				20	19	12	0.07232		
			-0.00588	0.00000	0.01117					0.04102	0.00000	-0.13171
			0.07472							0.11578		
			0.00000	-0.06997						0.00000	0.04311	
			0.03092	0.00000	-0.00475					0.05401	0.00000	-0.15889
23	26	20	-0.34498				22	25	19	-0.06017		
			0.16870	0.00000	-0.04579					0.20011	0.00000	0.24029
			1.02480							-0.31041		
			0.00000	-0.66048						0.00000	-0.55159	
			-0.67901	0.00000	-0.36432					-0.47790	0.00000	0.86200
24	23	20	0.09608				23	22	19	0.09338		
			0.01196	0.00000	0.11909					0.04224	0.00000	-0.11100
			-0.35816							0.25314		
			0.00000	0.02332						0.00000	-0.06804	
			-0.01271	0.00000	0.33484					0.03529	0.00000	-0.18510
26	27	28	0.99108				25	28	22	-0.04756		
			-0.04545	0.00000	0.11518					0.08296	0.00000	0.25051
			1.43003							0.08272		
			0.00000	-0.29777						0.00000	0.43486	
			0.94668	0.00000	-1.13226					0.00826	0.00000	-0.51758
27	26	28	-0.80614				26	25	28	0.03833		
			-0.02856	0.00000	-0.39517					-0.17029	0.00000	0.01539
			-0.39879							-0.00791		
			0.00000	0.42352						0.00000	-0.00806	
			0.11276	0.00000	-0.02473					-0.24567	0.00000	0.01597
28	26	29	-0.31901				28	30	25	-0.20835		
			0.10643	0.00000	0.12307					0.35255	0.00000	-0.24420
			-0.01365							2.05207		
			0.00000	-0.30408						0.00000	0.01907	
			0.16635	0.00000	0.31773					0.35806	0.00000	-2.07114
29	28	26	0.11913				29	28	25	0.16708		
			-0.05751	0.00000	-0.36677					0.25676	0.00000	-0.29883
			0.18164							0.30394		
			0.00000	0.12242						0.00000	0.03098	
			-0.07306	0.00000	-0.30406					0.22160	0.00000	-0.33492
							30	28	31	0.86373		
										0.00617	0.00000	0.05981
										0.64288		
										0.00000	0.45940	
										0.05239	0.00000	-1.10228
							31	30	32	-0.43183		
										-0.13876	0.00000	0.06794
										-0.09425		
										0.00000	-0.16794	
										-0.26538	0.00000	0.26219

							32	31	30	0.24013		
										-0.04341	0.00000	-0.32596
										0.20932		
										0.00000	0.10363	
										-0.04786	0.00000	-0.31295

S7.15 Lysine



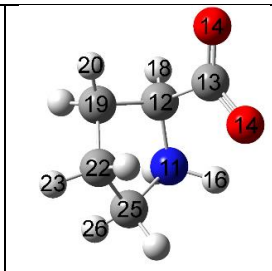
S7.16 Histidine



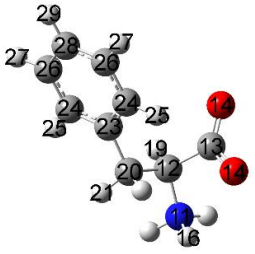
11	12	16	0.38053				11	12	16	0.34790		
			0.05370	0.00000	0.37636					-0.20084	0.00000	0.49353
			-0.53815							-1.05816		
			0.00000	-0.45595						0.00000	0.08709	
			0.17881	0.00000	0.99410					-0.24872	0.00000	0.97107
12	11	13	-0.35952				12	11	13	-0.42599		
			-0.27200	0.00000	0.36802					-0.28598	0.00000	0.33133
			-0.91721							-0.94970		
			0.00000	-0.06115						0.00000	0.26161	
			-0.84642	0.00000	0.97836					-0.76831	0.00000	0.68809
13	-14	-14	1.06417				13	-14	-14	1.01477		
			-0.00233	0.00000	-0.20372					0.06564	0.00000	-0.22231
			0.20679							-0.45356		
			0.00000	-0.34367						0.00000	-0.81456	
			-0.20701	0.00000	0.13688					-0.35788	0.00000	1.26812
14	13	14	-0.86799				14	13	14	-0.83563		
			0.26867	0.00000	-0.15087					0.15820	0.00000	-0.03499
			-0.62893							-0.72959		
			0.00000	0.15358						0.00000	0.13905	
			0.16289	0.00000	0.47535					0.07624	0.00000	0.59054
16	11	12	0.17804				16	11	12	0.20138		
			-0.02405	0.00000	-0.17036					0.01560	0.00000	-0.16708
			-0.15618							0.00872		
			0.00000	0.08092						0.00000	0.01238	
			-0.10798	0.00000	0.07526					0.07216	0.00000	-0.02110
19	12	11	0.06952				19	12	11	0.06349		
			-0.04577	0.00000	0.10104					-0.13834	0.00000	0.32669
			0.09120							-0.06418		
			0.00000	0.01905						0.00000	-0.16629	
			0.02135	0.00000	-0.11025					-0.13677	0.00000	0.23047
20	12	23	-0.09056				20	23	12	-0.07612		
			0.12741	0.00000	0.24825					0.38439	0.00000	0.30803
			-0.20130							-0.26913		
			0.00000	0.22679						0.00000	-0.66701	
			0.02757	0.00000	-0.02549					-0.08420	0.00000	0.93614
21	20	12	0.05029				21	20	12	0.09646		
			-0.02140	0.00000	-0.08875					-0.05139	0.00000	0.01069
			0.02259							-0.03066		
			0.00000	0.10111						0.00000	-0.08895	
			-0.01798	0.00000	-0.12370					-0.03737	0.00000	0.11961
23	-20	-26	-0.14293				23	30	24	0.19195		
			-0.04118	0.00000	0.27821					-0.20383	0.00000	0.39841
			0.34109							0.36031		
			0.00000	-0.39644						0.00000	-0.49158	

			-0.13797	0.00000	0.05535					0.30064	0.00000	0.13127
24	23	20	0.07968				24	26	23	-0.02399		
			-0.03375	0.00000	-0.05331					-0.06859	0.00000	0.33491
			-0.05293							-0.61566		
			0.00000	0.01761						0.00000	-0.81895	
			-0.07405	0.00000	0.03532					0.03547	0.00000	1.43461
26	29	23	-0.11383				25	24	26	0.04459		
			0.20668	0.00000	0.14313					0.01814	0.00000	-0.12114
			-0.02919							0.00479		
			0.00000	-0.39551						0.00000	-0.00163	
			0.22141	0.00000	0.42470					0.00379	0.00000	-0.00316
27	26	23	0.05568				26	28	24	-0.14139		
			0.01058	0.00000	-0.08142					0.20390	0.00000	0.02976
			0.04935							0.31740		
			0.00000	-0.13682						0.00000	-0.85788	
			0.07731	0.00000	0.08747					-0.43588	0.00000	0.54048
29	32	26	0.09488				27	26	24	0.12402		
			0.17635	0.00000	0.08680					-0.01886	0.00000	-0.25820
			-0.01224							0.02171		
			0.00000	0.02173						0.00000	0.05178	
			-0.65217	0.00000	-0.00949					-0.01200	0.00000	-0.07349
30	29	32	0.03229				28	30	26	0.33726		
			0.02138	0.00000	-0.12606					0.24742	0.00000	0.33036
			0.02356							0.44091		
			0.00000	0.03533						0.00000	-0.93448	
			-0.01860	0.00000	-0.05889					-0.44767	0.00000	0.49357
32	29	33	-0.32010				29	28	26	0.04548		
			-0.02706	0.00000	0.21691					-0.06414	0.00000	-0.11954
			-0.53231							0.01375		
			0.00000	-0.40679						0.00000	-0.01912	
			-0.13812	0.00000	0.93910					-0.06226	0.00000	0.00537
33	32	29	0.09191				30	28	23	-0.62777		
			-0.00900	0.00000	-0.40994					0.26776	0.00000	0.18089
			0.07013							-0.32995		
			0.00000	0.23251						0.00000	-0.26612	
			0.02574	0.00000	-0.30264					-0.05127	0.00000	0.59607

S7.17 Proline



S7.18 Phenylalanine

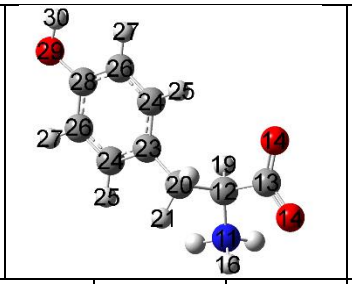


11	12	25	0.38214				11	12	16	0.34565		
			0.33339	0.00000	0.47882					0.04378	0.00000	0.33232
			-0.12654							0.51131		
			0.00000	-0.58041						0.00000	0.25437	
			0.12284	0.00000	0.70695					0.22697	0.00000	-0.76568
12	11	13	-0.42786				12	11	13	-0.26502		
			-0.23013	0.00000	0.49975					-0.19050	0.00000	0.31140
			-0.80902							-0.99749		

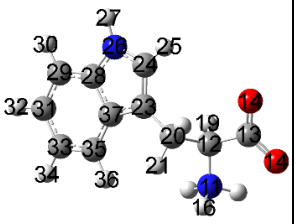
			0.00000	-0.59448						0.00000	-0.36013	
			-0.39185	0.00000	1.40350					-0.20688	0.00000	1.35762
13	-14	-14	1.02194				13	-14	-14	0.96343		
			0.16993	0.00000	-0.19397					0.22271	0.00000	-0.20501
			-0.43698							-0.62279		
			0.00000	-0.55369						0.00000	-0.69629	
			-0.39696	0.00000	0.99067					-0.45713	0.00000	1.31908
14	13	14	-0.84068				14	13	14	-0.85260		
			0.19915	0.00000	-0.06723					0.20930	0.00000	-0.11317
			-0.69691							-0.72121		
			0.00000	0.11658						0.00000	0.21087	
			0.13829	0.00000	0.58033					0.20500	0.00000	0.51034
16	11	12	0.18459				16	11	12	0.20503		
			-0.02091	0.00000	-0.14783					-0.07260	0.00000	-0.04855
			0.04317							0.00024		
			0.00000	0.02122						0.00000	-0.16869	
			-0.01853	0.00000	-0.06439					-0.06653	0.00000	0.16845
18	12	11	0.08331				19	12	11	-0.01057		
			-0.01528	0.00000	0.22785					-0.13412	0.00000	0.03623
			-0.12776							-0.05626		
			0.00000	-0.01831						0.00000	0.14216	
			0.00667	0.00000	0.14607					-0.21546	0.00000	-0.08590
19	12	22	-0.15368				20	23	12	-0.14333		
			0.32155	0.00000	0.27224					0.34039	0.00000	-0.02244
			0.34049							0.55306		
			0.00000	-0.42804						0.00000	0.84047	
			-0.31771	0.00000	0.08755					-0.88005	0.00000	-1.39353
20	19	12	0.09187				21	20	12	0.08864		
			-0.03215	0.00000	-0.01527					0.04326	0.00000	-0.15967
			-0.01019							0.02490		
			0.00000	-0.02359						0.00000	0.29855	
			-0.02200	0.00000	0.03378					0.02649	0.00000	-0.32345
22	25	19	-0.10299				23	-24	-24	-0.00558		
			0.36103	0.00000	0.38914					-0.00587	0.00000	-0.22496
			0.28691							-0.28301		
			0.00000	-0.59938						0.00000	-0.40686	
			0.00188	0.00000	0.31247					-0.20638	0.00000	0.68987
23	22	19	0.10673				24	23	26	0.04932		
			-0.01403	0.00000	-0.00953					0.14739	0.00000	0.08777
			-0.05105							-0.08330		
			0.00000	-0.00016						0.00000	-0.60316	
			-0.05496	0.00000	0.05121					-0.07188	0.00000	0.68646
25	11	22	-0.05350				25	24	23	-0.00275		
			0.26794	0.00000	0.56831					-0.05907	0.00000	-0.09417
			-0.09323							-0.16219		
			0.00000	-0.37662						0.00000	0.08720	
			0.06941	0.00000	0.46985					-0.00687	0.00000	0.07499
26	25	11	0.08281				26	-24	-28	-0.01621		
			-0.04445	0.00000	-0.01779					-0.00541	0.00000	0.08453
			-0.01683							0.37277		
			0.00000	0.01394						0.00000	-0.30255	
			-0.03181	0.00000	0.00289					-0.05948	0.00000	-0.07022
							27	26	24	-0.00077		
										-0.02549	0.00000	-0.17152
										0.07539		
										0.00000	-0.00481	
										-0.04932	0.00000	-0.07058
							28	-26	-26	-0.03011		
										-0.00746	0.00000	-0.03314
										0.38754		
										0.00000	-0.39878	
										0.30001	0.00000	0.01124

							29	28	26	-0.00082		
										-0.06395	0.00000	-0.12729
										0.01032		
										0.00000	-0.02081	
										-0.06005	0.00000	0.01049

S7.19 Tyrosine



S7.20 Tryptophane



11	12	16	0.41057				11	12	16	0.41080		
			-0.14311	0.00000	0.47719					0.02604	0.00000	0.44093
			0.34634							-0.07392		
			0.00000	0.25267						0.00000	0.30216	
			-0.31762	0.00000	-0.59901					0.21954	0.00000	-0.22824
12	11	13	-0.49186				12	11	13	-0.35582		
			0.08065	0.00000	0.18042					-0.30862	0.00000	0.32631
			-1.83071							-1.20667		
			0.00000	-1.83579						0.00000	-0.43290	
			-0.78006	0.00000	3.66650					-0.89523	0.00000	1.63957
13	-14	-14	1.10646				13	-14	-14	1.12098		
			0.02092	0.00000	-0.33643					0.03436	0.00000	-0.27598
			-0.19420							0.51537		
			0.00000	-0.83979						0.00000	-0.26924	
			-0.73251	0.00000	1.03399					-0.37883	0.00000	-0.24613
14	13	14	-0.84834				14	13	14	-0.84697		
			0.23198	0.00000	-0.03134					0.25295	0.00000	-0.13877
			-0.76074							-0.66175		
			0.00000	0.09011						0.00000	0.14532	
			0.18640	0.00000	0.67063					0.06563	0.00000	0.51643
16	11	12	0.11038				16	11	12	0.14508		
			-0.13957	0.00000	-0.13058					-0.08557	0.00000	-0.22928
			0.04627							0.13346		
			0.00000	-0.10943						0.00000	-0.07986	
			-0.17142	0.00000	0.06316					-0.06484	0.00000	-0.05360
19	12	11	-0.01327				19	12	11	0.05878		
			0.17640	0.00000	0.04014					-0.03347	0.00000	0.09038
			-0.22512							0.03928		
			0.00000	0.24982						0.00000	0.13596	
			0.12895	0.00000	-0.02470					-0.13283	0.00000	-0.17524
20	23	12	-0.07635				20	23	12	-0.27504		
			0.38383	0.00000	-0.02676					0.27806	0.00000	-0.34104
			0.29711							0.84973		
			0.00000	-1.94455						0.00000	-0.00887	
			0.84425	0.00000	1.64744					-0.35304	0.00000	-0.84086
21	20	12	0.07436				21	20	12	0.06684		
			-0.02829	0.00000	0.12567					0.01151	0.00000	-0.07764
			0.09674							-0.00313		
			0.00000	-0.56771						0.00000	0.04444	
			-0.01176	0.00000	0.47097					0.05459	0.00000	-0.04131
23	-24	-24	-0.04218				23	24	37	-0.04581		
			0.05437	0.00000	-0.31446					-0.36804	0.00000	-0.25494
			0.39782							0.15017		
			0.00000	-0.90248						0.00000	0.00798	

			1.52910	0.00000	0.50466					0.62457	0.00000	-0.15815
24	23	26	0.08953				24	26	23	0.05538		
			0.18702	0.00000	0.34963					-0.02516	0.00000	0.39982
			1.25210							-0.32120		
			0.00000	-1.27624						0.00000	-0.34253	
			0.48255	0.00000	0.02414					0.77765	0.00000	0.66373
25	24	23	-0.00327				25	24	26	0.01107		
			0.22957	0.00000	-0.10819					-0.06772	0.00000	-0.21185
			0.27152							-0.20109		
			0.00000	-0.09844						0.00000	0.21055	
			0.22401	0.00000	-0.17308					-0.26023	0.00000	-0.00946
26	28	24	-0.13615				26	28	24	-0.02408		
			-0.01964	0.00000	-0.19446					0.33931	0.00000	0.05558
			-0.73087							1.23475		
			0.00000	-0.15801						0.00000	-1.70676	
			-1.43438	0.00000	0.88888					1.27798	0.00000	0.47201
27	26	24	0.12419				27	26	24	0.14622		
			0.08549	0.00000	-0.16039					0.17400	0.00000	-0.11058
			0.04986							-0.17242		
			0.00000	0.01643						0.00000	0.10347	
			0.14376	0.00000	-0.06629					0.05311	0.00000	0.06895
28	29	26	0.34913				28	26	37	0.24382		
			-0.25734	0.00000	0.26053					-0.02630	0.00000	0.15376
			-0.94200							-0.04372		
			0.00000	-1.49108						0.00000	-0.38552	
			-1.26673	0.00000	2.43308					-0.12076	0.00000	0.42924
29	28	30	-0.43991				29	28	31	-0.13190		
			0.23412	0.00000	0.27272					-0.12140	0.00000	-0.04535
			-0.41697							0.92021		
			0.00000	-0.83211						0.00000	0.64441	
			-0.25240	0.00000	1.24908					0.08241	0.00000	-1.56462
30	29	28	0.26563				30	29	28	-0.00184		
			0.19812	0.00000	-0.14285					0.09970	0.00000	-0.22666
			0.07899							0.04360		
			0.00000	0.01855						0.00000	0.02355	
			0.31258	0.00000	-0.09754					0.37047	0.00000	-0.06715
							31	-29	-33	0.08506		
										0.03570	0.00000	0.54745
										-1.53711		
										0.00000	-1.40731	
										1.11613	0.00000	2.94442
							32	31	29	0.17530		
										-0.02279	0.00000	-0.00901
										0.01856		
										0.00000	0.04057	
										0.09768	0.00000	-0.05913
							33	-31	-35	-0.07673		
										-0.05003	0.00000	-0.04671
										-0.81319		
										0.00000	0.14432	
										-0.10232	0.00000	0.66887
							34	33	31	0.00829		
										-0.08767	0.00000	-0.33785
										0.12192		
										0.00000	0.13676	
										-0.15384	0.00000	-0.25868
							35	37	33	-0.22794		
										-0.09285	0.00000	-0.31531
										0.92353		
										0.00000	0.21213	
										-0.14857	0.00000	-1.13566
							36	35	33	-0.06294		

										0.17336	0.00000	-0.31559
										-0.02623		
										0.00000	0.19192	
										-0.07235	0.00000	-0.16569
							37	28	23	0.01142		
										-0.17883	0.00000	-0.18202
										-0.14250		
										0.00000	-0.01470	
										0.01056	0.00000	0.15720

REFERENCES FOR THE SI

1. E. V. Boldyreva, S. N. Ivashevskaya, H. Sowa, H. Ahsbahs and H. P. Weber, *Z. Kristallog.*, 2005, **220**, 50-57.
2. N. P. Funnell, W. G. Marshall and S. Parsons, *CrystEngComm*, 2011, **13**, 5841-5848.
3. B. Dalhus and C. H. Görbitz, *Acta Chem. Scand.*, 1996, **50**, 544-548.
4. C. H. Gorbitz and B. Dalhus, *Acta Cryst. C*, 1996, **52**, 1754-1756.
5. C. H. Gorbitz and B. Dalhus, *Acta Cryst. C*, 1996, **52**, 1464-1466.
6. B. A. Zakharov, B. A. Kolesov and E. V. Boldyreva, *Acta Cryst. B*, 2012, **68**, 275-286.
7. J. Janczak, D. Zobel and P. Luger, *Acta Cryst. C*, 1997, **53**, 1901-1904.
8. S. A. Moggach, S. J. Clark and S. Parsons, *Acta Cryst. E*, 2005, **61**, o2739-o2742.
9. E.-e. Bendeif and C. Jelsch, *Acta Cryst. C*, 2007, **63**, o361-o364.
10. K. Yamada, D. Hashizume, T. Shimizu and S. Yokoyama, *Acta Cryst. E*, 2007, **63**, o3802-o3803.
11. M. S. Lehmann and A. C. Nunes, *Acta Cryst. B*, 1980, **36**, 1621-1625.
12. P. Lozano-Casal, D. R. Allan and S. Parsons, *Acta Cryst. B*, 2008, **64**, 466-475.
13. E. Courvoisier, P. A. Williams, G. K. Lim, C. E. Hughes and K. D. M. Harris, *ChemComm*, 2012, **48**, 2761-2763.
14. P. A. Williams, C. E. Hughes and K. D. M. Harris, *Angew. Chem.*, 2015, **127**, 4045-4049.
15. J. J. Madden, N. C. Seeman and E. L. McGandy, *Acta Cryst. B*, 1972, **B 28**, 2377-2382.
16. R. L. Kayushina and Vainshte.Kb, *Sov. Phys. - Crystallogr.*, 1966, **10**, 698.
17. F. S. Ihlefeldt, F. B. Pettersen, A. von Bonin, M. Zawadzka and C. H. Gorbitz, *Angew. Chem. Int. Edit.*, 2014, **53**, 13600-13604.
18. M. N. Frey, T. F. Koetzle, M. S. Lehmann and W. C. Hamilton, *J. Chem. Phys.*, 1973, **58**, 2547-2556.
19. C. H. Gorbitz, K. W. Tornroos and G. M. Day, *Acta Cryst. B*, 2012, **68**, 549-557.
20. V. A. Drebushchak, Y. A. Kovalevskaya, I. E. Paukov and E. V. Boldyreva, *J. Therm. Anal. Calorim.*, 2003, **74**, 109-120.
21. H. M. Huffman and H. Borsook, *J. Am. Chem. Soc.*, 1932, **54**, 4297-4301.
22. J. O. Hutchens, A. G. Cole and J. W. Stout, *J. Am. Chem. Soc.*, 1960, **82**, 4813-4815.
23. J. O. Hutchens, A. G. Cole and J. W. Stout, *J. Phys. Chem.*, 1963, **67**, 1128-1130.
24. J. O. Hutchens, R. A. Robie, A. G. Cole and J. W. Stout, *J. Biol. Chem.*, 1963, **238**, 2407-&.
25. H. M. Huffman and E. L. Ellis, *J. Am. Chem. Soc.*, 1937, **59**, 2150-2152.
26. J. O. Hutchens, A. G. Cole and J. W. Stout, *J. Biol. Chem.*, 1964, **239**, 4194-4195.
27. A. G. Cole, J. O. Hutchens and J. W. Stout, *J. Phys. Chem.*, 1963, **67**, 1852-1855.
28. I. E. Paukov, Y. A. Kovalevskaya and E. V. Boldyreva, *J. Therm. Anal. Calorim.*, 2010, **100**, 295-301.
29. J. O. Hutchens, J. W. Stout and A. G. Cole, *J. Biol. Chem.*, 1964, **239**, 591-595.

30. O. V. Dorofeeva and O. N. Ryzhova, *The Journal of Physical Chemistry A*, 2014, **118**, 3490-3502.
1. E. V. Boldyreva, S. N. Ivashevskaya, H. Sowa, H. Ahsbahs and H. P. Weber, *Z. Kristallog.*, 2005, **220**, 50-57.
2. N. P. Funnell, W. G. Marshall and S. Parsons, *CrystEngComm*, 2011, **13**, 5841-5848.
3. B. Dalhus and C. H. Görbitz, *Acta Chem. Scand.*, 1996, **50**, 544-548.
4. C. H. Gorbitz and B. Dalhus, *Acta Cryst. C*, 1996, **52**, 1754-1756.
5. C. H. Gorbitz and B. Dalhus, *Acta Cryst. C*, 1996, **52**, 1464-1466.
6. B. A. Zakharov, B. A. Kolesov and E. V. Boldyreva, *Acta Cryst. B*, 2012, **68**, 275-286.
7. J. Janczak, D. Zobel and P. Luger, *Acta Cryst. C*, 1997, **53**, 1901-1904.
8. S. A. Moggach, S. J. Clark and S. Parsons, *Acta Cryst. E*, 2005, **61**, o2739-o2742.
9. E.-e. Bendeif and C. Jelsch, *Acta Cryst. C*, 2007, **63**, o361-o364.
10. K. Yamada, D. Hashizume, T. Shimizu and S. Yokoyama, *Acta Cryst. E*, 2007, **63**, o3802-o3803.
11. M. S. Lehmann and A. C. Nunes, *Acta Cryst. B*, 1980, **36**, 1621-1625.
12. P. Lozano-Casal, D. R. Allan and S. Parsons, *Acta Cryst. B*, 2008, **64**, 466-475.
13. E. Courvoisier, P. A. Williams, G. K. Lim, C. E. Hughes and K. D. M. Harris, *ChemComm*, 2012, **48**, 2761-2763.
14. P. A. Williams, C. E. Hughes and K. D. M. Harris, *Angew. Chem.*, 2015, **127**, 4045-4049.
15. J. J. Madden, N. C. Seeman and E. L. McGandy, *Acta Cryst. B*, 1972, **B 28**, 2377-2382.
16. R. L. Kayushina and Vainshte.Kb, *Sov. Phys. - Crystallogr.*, 1966, **10**, 698.
17. F. S. Ihlefeldt, F. B. Pettersen, A. von Bonin, M. Zawadzka and C. H. Gorbitz, *Angew. Chem. Int. Edit.*, 2014, **53**, 13600-13604.
18. M. N. Frey, T. F. Koetzle, M. S. Lehmann and W. C. Hamilton, *J. Chem. Phys.*, 1973, **58**, 2547-2556.
19. C. H. Gorbitz, K. W. Tornroos and G. M. Day, *Acta Cryst. B*, 2012, **68**, 549-557.
20. V. A. Drebushchak, Y. A. Kovalevskaya, I. E. Paukov and E. V. Boldyreva, *J. Therm. Anal. Calorim.*, 2003, **74**, 109-120.
21. H. M. Huffman and H. Borsook, *J. Am. Chem. Soc.*, 1932, **54**, 4297-4301.
22. J. O. Hutchens, A. G. Cole and J. W. Stout, *J. Am. Chem. Soc.*, 1960, **82**, 4813-4815.
23. J. O. Hutchens, A. G. Cole and J. W. Stout, *J. Phys. Chem.*, 1963, **67**, 1128-1130.
24. J. O. Hutchens, R. A. Robie, A. G. Cole and J. W. Stout, *J. Biol. Chem.*, 1963, **238**, 2407-&.
25. H. M. Huffman and E. L. Ellis, *J. Am. Chem. Soc.*, 1937, **59**, 2150-2152.
26. J. O. Hutchens, A. G. Cole and J. W. Stout, *J. Biol. Chem.*, 1964, **239**, 4194-4195.
27. A. G. Cole, J. O. Hutchens and J. W. Stout, *J. Phys. Chem.*, 1963, **67**, 1852-1855.
28. I. E. Paukov, Y. A. Kovalevskaya and E. V. Boldyreva, *J. Therm. Anal. Calorim.*, 2010, **100**, 295-301.
29. J. O. Hutchens, J. W. Stout and A. G. Cole, *J. Biol. Chem.*, 1964, **239**, 591-595.