Table 9.5.1.1. *Average lengths (Å) for bonds involving the elements H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, and I*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
As(3)—As(3)	X_2—**As**—**As**—X_2	2.459	2.457	0.011	2.456	2.466	8	
As—B	see CUDLOC (2.065), CUDLUI (2.041)							
As—Br	see CODDEE, CODDII (2.346–3.203)							
As(4)—C	X_3—**As**—**C**H_3 $(X)_2$(C, O, S=)**As**—**C**sp^3 **As**—**C**$_{ar}$ in Ph_4As^+ $(X)_2$(C, O, S=)**As**—**C**$_{ar}$	1.903 1.927 1.905 1.922	1.907 1.929 1.909 1.927	0.016 0.017 0.012 0.016	1.893 1.921 1.897 1.908	1.916 1.937 1.912 1.934	12 16 108 36	
As(3)—C	X_2—**As**—**C**sp^3 X_2—**As**—**C**$_{ar}$	1.963 1.956	1.965 1.956	0.017 0.015	1.948 1.944	1.978 1.964	6 41	
As(3)—Cl	X_2—**As**—**Cl**	2.268	2.256	0.039	2.247	2.281	10	
As(6)—F	in **As**F_6^-	1.678	1.676	0.020	1.659	1.695	36	
As(3)—I	see OPIMAS (2.579, 2.590)							
As(3)—N(3)	X_2—**As**—**N**—X_2	1.858	1.858	0.029	1.839	1.873	19	
As(4)=N(2)	see TPASSN (1.837)							
As(4)—O	$(X)_2$(O=)**As**—**O**H	1.710	1.712	0.017	1.695	1.726	6	
As(3)—O	see ASAZOC, PHASOC01 (1.787–1.845)							
As(4)=O	X_3—**As**=**O**	1.661	1.661	0.016	1.652	1.667	9	
As(3)—P(3)	see BELNIP (2.350, 2.362)							†
As(3)=P(3)	see BUTHAZ10 (2.124)							†
As(3)—S	X_2—**As**—**S**	2.275	2.266	0.032	2.247	2.298	14	
As(4)=S	X_3—**As**=**S**	2.083	2.082	0.004	2.080	2.086	9	
As(3)—Se(2)	see COSDIX, ESEARS (2.355–2.401)							†
As(3)—Si(4)	see BICGEZ, MESIAD (2.351–2.365)							†
As(3)—Te(2)	see ETEARS (2.571, 2.576)							†
B(*n*)—B(*n*)	*n* = 5–7 in boron cages	1.775	1.773	0.031	1.763	1.786	688	
B(4)—B(4)	see CETTAW (2.041)							
B(4)—B(3)	see COFVOI (1.698)							
B(3)—B(3)	X_2—**B**—**B**—X_2	1.701	1.700	0.014	1.691	1.712	8	
B(6)—Br		1.967	1.971	0.014	1.954	1.979	7	†
B(4)—Br		2.017	2.008	0.031	1.990	2.044	15	†
B(*n*)—C	*n* = 5–7: **B**—**C** in cages *n* = 3–4: **B**—**C**sp^3 not cages *n* = 4: **B**—**C**$_{ar}$ **B**$^-$—**C**$_{ar}$ in Ph_4B^- *n* = 3: **B**—**C**$_{ar}$	1.716 1.597 1.606 1.643 1.556	1.717 1.599 1.607 1.643 1.552	0.020 0.022 0.012 0.006 0.015	1.707 1.585 1.596 1.641 1.546	1.728 1.611 1.615 1.645 1.566	96 29 41 16 24	*1*
B(*n*)—Cl	**B**(5)—**Cl** and **B**(3)—**Cl** **B**(4)—**Cl**	1.751 1.833	1.751 1.833	0.011 0.013	1.743 1.821	1.761 1.843	14 22	
B(4)—F	**B**—**F** (B neutral) **B**$^-$—**F** in BF_4^-	1.366 1.365	1.368 1.372	0.017 0.029	1.356 1.352	1.375 1.390	25 84	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
B(4)—I	see TMPBTI (2.220, 2.253)							
B(4)—N(3)	X_3—**B**—**N**(=C)(*X*) in pyrazaboles	1.611 1.549	1.617 1.552	0.013 0.015	1.601 1.536	1.625 1.560	8 10	
B(3)—N(3)	X_2—**B**—**N**—C_2: all coplanar for τ(BN) > 30° see BOGSUL, BUSHAY, CILRUK (1.434–1.530) S_2—**B**—**N**—X_2	1.404 1.447	1.404 1.443	0.014 0.013	1.389 1.435	1.408 1.470	40 14	*2*
B(4)—O	**B**—**O** in BO_4^- for neutral **B**—**O** see Note 3	1.468	1.468	0.022	1.453	1.479	24	*3*
B(3)—O(2)	X_2—**B**—**O**—*X*	1.367	1.367	0.024	1.349	1.382	35	
B(*n*)—P	*n* = 4: **B**—**P** *n* = 3: see BUPSIB10 (1.892, 1.893)	1.922	1.927	0.027	1.900	1.954	10	
B(4)—S	**B**(4)—**S**(3) **B**(4)—**S**(2)	1.930 1.896	1.927 1.896	0.009 0.004	1.925 1.893	1.934 1.899	10 6	
B(3)—S	N—**B**—$\mathbf{S}_2$ (=*X*—)(N—)**B**—**S**	1.806 1.851	1.806 1.854	0.010 0.013	1.799 1.842	1.816 1.859	28 10	
Br—Br	see BEPZEB, TPASTB	2.542	2.548	0.015	2.526	2.551	4	
Br—C	**Br**—**C*** **Br**—C*sp*^{3} (cyclopropane) **Br**—C*sp*^{2} **Br**—$\mathbf{C}_{ar}$ (mono-Br + *m*,*p*-Br_2) **Br**—$\mathbf{C}_{ar}$ (*o*-Br_2)	1.966 1.910 1.883 1.899 1.875	1.967 1.910 1.881 1.899 1.872	0.029 0.010 0.015 0.012 0.011	1.951 1.900 1.874 1.892 1.864	1.983 1.914 1.894 1.906 1.884	100 8 31 119 8	*4* *4* *4* *4*
$^-$Br(2)—Cl	see TEACBR (2.362–2.402)							†
Br—I	see DTHIBR10 (2.646), TPHOSI (2.695)							
Br—N	see NBBZAM (1.843)							
Br—O	see CIYFOF	1.581	1.581	0.007	1.574	1.587	4	
Br—P	see CISTED (2.366)							
Br—S(2)	see BEMLIO (2.206)							†
Br—S(3)	see CIWYIQ (2.435, 2.453)							†
Br—S(3)$^+$	see THINBR (2.321)							†
Br—Se	see CIFZUM (2.508, 2.619)							
Br—Si	see BIZJAV (2.284)							
Br—Te	In $\mathbf{Br}_6\mathbf{Te}^{2-}$ see CUGBAH (2.692–2.716) **Br**—**Te**(4) see BETUTE10 (3.079, 3.015) **Br**—**Te**(3) see BTUPTE (2.835)							
C*sp*^{3}—C*sp*^{3}	C$^\#$—$\mathbf{CH}_2$—$\mathbf{CH}_3$ $(C^\#)_2$—**C**H—$\mathbf{CH}_3$ $(C^\#)_3$—**C**—$\mathbf{CH}_3$ C$^\#$—$\mathbf{CH}_2$—$\mathbf{CH}_2$—C$^\#$ $(C^\#)_2$—**C**H—$\mathbf{CH}_2$—C$^\#$ $(C^\#)_3$—**C**—$\mathbf{CH}_2$—C$^\#$ $(C^\#)_2$—**C**H—**C**H—$(C^\#)_2$ $(C^\#)_3$—**C**—**C**H—$(C^\#)_2$ $(C^\#)_3$—**C**—**C**—$(C^\#)_3$ **C***—**C*** (overall)	1.513 1.524 1.534 1.524 1.531 1.538 1.542 1.556 1.588 1.530	1.514 1.526 1.534 1.524 1.531 1.539 1.542 1.556 1.580 1.530	0.014 0.015 0.011 0.014 0.012 0.010 0.011 0.011 0.025 0.015	1.507 1.518 1.527 1.516 1.524 1.533 1.536 1.549 1.566 1.521	1.523 1.534 1.541 1.532 1.538 1.544 1.549 1.562 1.610 1.539	192 226 825 2459 1217 330 321 215 21 5777	*5, 6*

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	d	m	σ	q_l	q_u	n	Note
Csp^3—Csp^3 (*cont.*)	in cyclopropane (any substituent)	1.510	1.509	0.026	1.497	1.523	888	*7*
	in cyclobutane (any substituent)	1.554	1.553	0.021	1.540	1.567	679	*8*
	in cyclopentane (C,H substituents)	1.543	1.543	0.018	1.532	1.554	1641	
	in cyclohexane (C,H substituents)	1.535	1.535	0.016	1.525	1.545	2814	
	cyclopropyl—C* (exocyclic)	1.518	1.518	0.019	1.505	1.531	366	*7*
	cyclobutyl—C* (exocyclic)	1.529	1.529	0.016	1.519	1.539	376	*8*
	cyclopentyl—C* (exocyclic)	1.540	1.541	0.017	1.527	1.549	956	
	cyclohexyl—C* (exocyclic)	1.539	1.538	0.016	1.529	1.549	2682	
	in cyclobutene (any substituent)	1.573	1.574	0.017	1.566	1.586	25	*8*
	in cyclopentene (C,H substituents)	1.541	1.539	0.015	1.532	1.549	208	
	in cyclohexene (C,H substituents)	1.541	1.541	0.020	1.528	1.554	586	
	in oxirane (epoxide)	1.466	1.466	0.015	1.458	1.474	249	*9*
	in aziridine	1.480	1.481	0.021	1.465	1.496	67	*9*
	in oxetane	1.541	1.541	0.019	1.527	1.557	16	
	in azetidine	1.548	1.543	0.018	1.536	1.558	22	
	oxiranyl—C* (exocyclic)	1.509	1.507	0.018	1.497	1.519	333	*9*
	aziridinyl—C* (exocyclic)	1.512	1.512	0.018	1.496	1.526	13	*9*
Csp^3—Csp^2	**C**H_3—**C**=C	1.503	1.504	0.011	1.497	1.509	215	
	C$^{\#}$—**C**H_2—**C**=C	1.502	1.502	0.013	1.494	1.510	483	
	(C$^{\#}$)$_2$—**C**H—**C**=C	1.510	1.510	0.014	1.501	1.518	564	
	(C$^{\#}$)$_3$—**C**—**C**=C	1.522	1.522	0.016	1.511	1.533	193	
	C*—**C**=C (overall)	1.507	1.507	0.015	1.499	1.517	1456	*5*
	C*—**C**=C (endocylic):							
	in cyclopropene	1.509	1.508	0.016	1.500	1.516	20	*10*
	in cyclobutene	1.513	1.512	0.018	1.500	1.525	50	*8*
	in cyclopentene	1.512	1.512	0.014	1.502	1.521	208	
	in cyclohexene	1.506	1.505	0.016	1.495	1.516	391	
	in cyclopentadiene	1.502	1.503	0.019	1.490	1.515	18	
	in cyclohexa-1,3-diene	1.504	1.504	0.017	1.491	1.517	56	
	C*—**C**≡C (exocyclic):							
	cyclopropenyl—C*	1.478	1.475	0.012	1.470	1.485	7	*10*
	cyclobutenyl—C*	1.489	1.483	0.015	1.479	1.496	11	*8*
	cyclopentenyl—C*	1.504	1.506	0.012	1.495	1.512	115	
	cyclohexenyl—C*	1.511	1.511	0.013	1.502	1.519	292	
	C*—**C**H=O in aldehydes	1.510	1.510	0.008	1.501	1.518	7	
	(**C***)$_2$—**C**=O in ketones	1.511	1.511	0.015	1.501	1.521	952	*11*
	in cyclobutanone	1.529	1.530	0.016	1.514	1.545	18	
	in cyclopentanone	1.514	1.514	0.016	1.505	1.523	312	
	acyclic and 6+ rings	1.509	1.509	0.016	1.499	1.519	626	
	C*—**C**OOH in carboxylic acids	1.502	1.502	0.014	1.495	1.510	176	
	C*—**C**OO$^-$ in carboxylate anions	1.520	1.521	0.011	1.516	1.528	57	
	C*—**C**(=O)(—OC*) in acyclic esters	1.497	1.496	0.018	1.484	1.509	553	*12*
	in β-lactones	1.519	1.519	0.020	1.500	1.538	4	*13*
	in γ-lactones	1.512	1.512	0.015	1.501	1.521	110	*12*
	in δ-lactones	1.504	1.502	0.013	1.495	1.517	27	*12*
	cyclopropyl (**C**)—**C**=O in ketones, acids, and esters	1.486	1.485	0.018	1.474	1.497	105	*7*
	C*—**C**(=O)(—NH_2) in acyclic amides	1.514	1.512	0.016	1.506	1.526	32	*14*
	C*—**C**(=O)(—NHC*) in acyclic amides	1.506	1.505	0.012	1.498	1.515	78	*14*
	C*—**C**(=O)[—N(C*)$_2$] in acyclic amides	1.505	1.505	0.011	1.496	1.517	15	*14*
Csp^3—C$_{ar}$	**C**H_3—**C**$_{ar}$	1.506	1.507	0.011	1.501	1.513	454	
	C$^{\#}$—**C**H_2—**C**$_{ar}$	1.510	1.510	0.009	1.505	1.516	674	
	(C$^{\#}$)$_2$—**C**—**C**$_{ar}$	1.515	1.515	0.011	1.508	1.522	363	
	(C$^{\#}$)$_3$—**C**—**C**$_{ar}$	1.527	1.530	0.016	1.517	1.539	308	
	C*—**C**$_{ar}$ (overall)	1.513	1.513	0.014	1.505	1.521	1813	
	cylopropyl (**C**)—**C**$_{ar}$	1.490	1.490	0.015	1.479	1.503	90	*7*

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
C*sp*^{3}—C*sp*^{1}	**C***—**C**≡C	1.466	1.465	0.010	1.460	1.469	21	*15*
	C$^{\#}$—**C**≡C	1.472	1.472	0.012	1.464	1.481	88	*15*
	C*—**C**≡N	1.470	1.469	0.013	1.463	1.479	106	*7(b)*
	cyclopropyl (**C**)—**C**≡N	1.444	1.447	0.010	1.436	1.451	38	*7*
C*sp*^{2}—C*sp*^{2}	C=**C**—**C**=C (conjugated)	1.455	1.455	0.011	1.447	1.463	30	*16, 18*
	(unconjugated)	1.478	1.476	0.012	1.470	1.479	8	*17, 18*
	(overall)	1.460	1.460	0.015	1.450	1.470	38	
	C=**C**—**C**=**C**—**C**=C	1.443	1.445	0.013	1.431	1.454	29	*18*
	C=**C**—**C**=C (endocyclic in TCNQ)	1.432	1.433	0.012	1.424	1.441	280	*19*
	C=**C**—**C**(=O)(—C*) (conjugated)	1.464	1.462	0.018	1.453	1.476	211	*16, 18*
	(unconjugated)	1.484	1.486	0.017	1.475	1.497	14	*17, 18*
	(overall)	1.465	1.462	0.018	1.453	1.478	226	
	C=**C**—**C**(=O)—**C**=C:							
	in benzoquinone (C,H substituents only)	1.478	1.476	0.011	1.469	1.488	28	
	in benzoquinone (any substituent)	1.478	1.478	0.031	1.464	1.498	172	
	non-quinonoid	1.456	1.455	0.012	1.447	1.464	28	
	C—**C**—COOH	1.475	1.476	0.015	1.461	1.488	22	
	C=**C**—COOC*	1.488	1.489	0.014	1.478	1.497	113	
	C=**C**—COO$^-$	1.502	1.499	0.017	1.488	1.510	11	
	HOO**C**—COOH	1.538	1.537	0.007	1.535	1.541	9	
	HOO**C**—COO$^-$	1.549	1.552	0.009	1.546	1.553	13	
	$^-$OO**C**—COO$^-$	1.564	1.559	0.022	1.554	1.568	9	
	formal C*sp*^{2}—C*sp*^{2} single bond in selected, non-fused heterocycles:							
	in 1*H*-pyrrole (C3—C4)	1.412	1.410	0.016	1.401	1.427	29	
	in furan (C3—C4)	1.423	1.423	0.016	1.412	1.433	62	
	in thiophene (C3—C4)	1.424	1.425	0.015	1.415	1.433	40	
	in pyrazole (C3—C4)	1.410	1.412	0.016	1.400	1.418	20	
	in isoxazole (C3—C4)	1.425	1.425	0.016	1.413	1.438	9	
	in furazan (C3—C4)	1.428	1.427	0.007	1.422	1.435	6	
	in furoxan (C3—C4)	1.417	1.417	0.006	1.412	1.422	14	
C*sp*^{2}—C$_{ar}$	C=**C**—**C**$_{ar}$ (conjugated)	1.470	1.470	0.015	1.463	1.480	37	*16, 18*
	(unconjugated)	1.488	1.490	0.012	1.480	1.496	87	*17, 18*
	(overall)	1.483	1.483	0.015	1.472	1.494	124	
	cyclopropenyl (C=**C**)—**C**$_{ar}$	1.447	1.448	0.006	1.441	1.452	8	*10*
	C$_{ar}$—**C**(=O)—C*	1.488	1.489	0.016	1.478	1.500	84	
	C$_{ar}$—**C**(=O)—**C**$_{ar}$	1.480	1.481	0.017	1.468	1.494	58	
	C$_{ar}$—COOH	1.484	1.485	0.014	1.474	1.491	75	
	C$_{ar}$—**C**(=O)(—OC*)	1.487	1.487	0.012	1.480	1.494	218	
	C$_{ar}$—COO$^-$	1.504	1.509	0.014	1.495	1.512	26	
	C$_{ar}$—**C**(=O)—NH$_2$	1.500	1.503	0.020	1.498	1.510	19	
	C$_{ar}$—**C**=N—C$^{\#}$ (conjugated)	1.476	1.478	0.014	1.466	1.486	27	*16*
	(unconjugated)	1.491	1.490	0.008	1.485	1.496	48	*17*
	(overall)	1.485	1.487	0.013	1.481	1.493	75	
	in indole (C3—C3a)	1.434	1.434	0.011	1.428	1.439	40	
C*sp*^{2}—C*sp*^{1}	C=**C**—**C**≡C	1.431	1.427	0.014	1.425	1.441	11	*7(b)*
	C=**C**—**C**≡N in TCNQ	1.427	1.427	0.010	1.420	1.433	280	*19*
C$_{ar}$—C$_{ar}$	in biphenyls (*ortho* substituent all H)	1.487	1.488	0.007	1.484	1.493	30	
	(≥ 1 non-H *ortho* substituent)	1.490	1.491	0.010	1.486	1.495	212	
C$_{ar}$—C*sp*^{1}	**C**$_{ar}$—**C**≡C	1.434	1.436	0.006	1.430	1.437	37	
	C$_{ar}$—**C**≡N	1.443	1.444	0.008	1.436	1.448	31	
C*sp*^{1}—C*sp*^{1}	C≡**C**—**C**≡C	1.377	1.378	0.012	1.374	1.384	21	
C*sp*^{2}=C*sp*^{2}	C*—**C**H=**C**H$_2$	1.299	1.300	0.027	1.280	1.311	42	
	(C*)$_2$—**C**=**C**H$_2$	1.321	1.321	0.013	1.313	1.328	77	
	C*—**C**H=**C**H—C* (*cis*)	1.317	1.318	0.013	1.310	1.323	106	
	(*trans*)	1.312	1.311	0.011	1.304	1.320	19	
	(overall)	1.316	1.317	0.015	1.309	1.323	127	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
Csp^2=Csp^2 (*cont.*)	(C*)$_2$—**C**=**C**H—C*	1.326	1.328	0.011	1.319	1.334	168	
	(C*)$_2$—**C**=**C**—(C*)$_2$	1.331	1.330	0.009	1.326	1.334	89	
	(C*,H)$_2$—**C**=**C**—(C*,H)$_2$ (overall)	1.322	1.323	0.014	1.315	1.331	493	*5*
	in cyclopropene (any substituent)	1.294	1.288	0.017	1.284	1.302	10	*10*
	in cyclobutene (any substituent)	1.335	1.335	0.019	1.324	1.347	25	*8*
	in cyclopentene (C,H substituents)	1.323	1.324	0.013	1.314	1.331	104	
	in cyclohexene (C,H substituents)	1.326	1.325	0.012	1.318	1.334	196	
	C=**C**=**C** (allenes, any substituents)	1.307	1.307	0.005	1.303	1.310	18	
	C=**C**—**C**=**C** (C,H substituents, conjugated)	1.330	1.330	0.014	1.322	1.338	76	*16*
	C=**C**—**C**=**C**—**C**=**C** (C,H substituents, conjugated)	1.345	1.345	0.012	1.337	1.350	58	*16*
	C=**C**—C$_{ar}$ (C,H substituents, conjugated)	1.339	1.340	0.011	1.334	1.346	124	*16*
	C=**C** in cyclopenta-1,3-diene (any substituent)	1.341	1.341	0.017	1.328	1.356	18	
	C=**C** in cyclohexa-1,3-diene (any substituent)	1.332	1.332	0.013	1.323	1.341	56	
	in **C**=**C**—C=O (C,H substituent, conjugated)	1.340	1.340	0.013	1.332	1.348	211	*16, 18*
	(C,H substituent, unconjugated)	1.331	1.330	0.008	1.326	1.339	14	*17, 18*
	(C,H substituent, overall)	1.340	1.339	0.013	1.332	1.348	226	
	in cyclohexa-2,5-dien-1-ones	1.329	1.327	0.011	1.321	1.335	28	
	in *p*-benzoquinones (C*,H substituents)	1.333	1.337	0.011	1.325	1.338	14	
	(any substituent)	1.349	1.339	0.030	1.330	1.364	86	
	in TCNQ (endocyclic)	1.352	1.353	0.010	1.345	1.358	142	*19*
	(exocyclic)	1.392	1.391	0.017	1.379	1.405	139	*19*
	C=**C**—OH in enol tautomers	1.362	1.360	0.020	1.349	1.370	54	
	in heterocycles (any substituent)							
	1*H*-pyrrole (C2—C3, C4—C5)	1.375	1.377	0.018	1.361	1.388	58	
	furan (C2—C3, C4—C5)	1.341	1.342	0.021	1.329	1.351	125	
	thiophene (C2—C3, C4—C5)	1.362	1.359	0.025	1.346	1.377	60	
	pyrazole (C4—C5)	1.369	1.372	0.019	1.362	1.383	20	
	imidazole (C4—C5)	1.360	1.361	0.014	1.352	1.367	44	
	isoxazole (C4—C5)	1.341	1.336	0.012	1.331	1.355	9	
	indole (C2—C3)	1.364	1.363	0.012	1.355	1.371	40	
C$_{ar}$ ⋯ C$_{ar}$	in phenyl rings with C*,H substituents only:							
	H—**C**⋯**C**—H	1.380	1.381	0.013	1.372	1.388	2191	
	C*—**C**⋯**C**—H	1.387	1.388	0.010	1.382	1.393	891	
	C*—**C**⋯**C**—C*	1.397	1.397	0.009	1.392	1.403	182	
	C⋯**C** (overall)	1.384	1.384	0.013	1.375	1.391	3264	
	F—**C**⋯**C**—F	1.372	1.374	0.011	1.366	1.380	84	*4*
	Cl—**C**⋯**C**—Cl	1.388	1.389	0.014	1.380	1.398	152	*4*
	in napthalene (D_{2h}) C1—C2	1.364	1.364	0.014	1.356	1.373	440	
	(any substituent) C2—C3	1.406	1.406	0.014	1.397	1.415	218	
	C1—C8a	1.420	1.419	0.012	1.412	1.426	440	
	C4a—C8a	1.422	1.424	0.011	1.417	1.429	109	
	in anthracene (D_{2h}) C1—C2	1.356	1.356	0.009	1.350	1.360	56	
	(any substituent) C2—C3	1.410	1.410	0.010	1.401	1.416	34	
	C1—C9a	1.430	1.430	0.006	1.426	1.434	56	
	C4a—C9a	1.435	1.436	0.007	1.429	1.440	34	
	C9—C9a	1.400	1.402	0.009	1.395	1.406	68	
	in pyridine (C,H substituent)	1.379	1.381	0.012	1.371	1.387	276	*20*
	(any substituents)	1.380	1.380	0.015	1.371	1.389	537	*20*
	in pyridinium cation:							
	(N^+—H; C,H substituents on C) C2—C3	1.373	1.375	0.012	1.368	1.380	30	
	C3—C4	1.379	1.380	0.011	1.371	1.388	30	
	(N^+—*X*; C,H substituents on C) C2—C3	1.373	1.372	0.019	1.362	1.382	151	
	C3—C4	1.383	1.385	0.019	1.372	1.394	151	
	in pyrazine (H substituent on C)	1.379	1.377	0.010	1.370	1.388	10	
	(any substituent on C)	1.405	1.405	0.024	1.388	1.420	60	
	in pyrimidine (C,H substituents on C)	1.387	1.389	0.018	1.379	1.400	28	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
Csp^1≡Csp^1	*X*—**C**≡**C**—*X*	1.183	1.183	0.014	1.174	1.193	119	*15*
	C,H—**C**≡**C**—C,H	1.181	1.181	0.014	1.173	1.192	104	*15*
	in **C**≡**C**—C(sp^2, ar)	1.189	1.193	0.010	1.181	1.195	38	*15*
	in **C**≡**C**—**C**≡**C**	1.192	1.192	0.010	1.187	1.197	42	*15*
	in **C**H≡**C**—C#	1.174	1.174	0.011	1.167	1.180	42	*15*
Csp^3—Cl	Omitting 1,2-dichlorides:							
	C—**C**H_2—**Cl**	1.790	1.790	0.007	1.783	1.795	13	*4*
	C_2—**C**H—**Cl**	1.803	1.802	0.003	1.800	1.807	8	*4*
	C_3—**C**—**Cl**	1.849	1.856	0.011	1.837	1.858	5	*4*
	X—**C**H_2—**Cl** (*X* = C,H,N,O)	1.790	1.791	0.011	1.783	1.797	37	*4*
	X_2—**C**H—**Cl** (*X* = C,H,N,O)	1.805	1.803	0.014	1.800	1.812	26	*4*
	X_3—**C**—**Cl** (*X* = C,H,N,O)	1.843	1.838	0.014	1.835	1.858	7	*4*
	X_2—**C**—**C**l_2 (*X* = C,H,N,O)	1.779	1.776	0.015	1.769	1.790	18	*4*
	X—**C**—**C**l_3 (*X* = C,H,N,O)	1.768	1.765	0.011	1.761	1.776	33	*4*
	Cl—CH(—C)—**C**H(—C)—**Cl**	1.793	1.793	0.013	1.786	1.800	66	*4*
	Cl—**C**(—C_2)—**C**(—C_2)—**Cl**	1.762	1.760	0.010	1.757	1.765	54	*4*
	cyclopropyl—Cl	1.755	1.756	0.011	1.749	1.763	64	
Csp^2—Cl	C=**C**—**Cl** (C,H,N,O substituents on C)	1.734	1.729	0.019	1.719	1.748	63	*4*
	C=**C**—**C**l_2 (C,H,N,O substituents on C)	1.720	1.716	0.013	1.708	1.729	20	*4*
	Cl—**C**=**C**—**Cl**	1.713	1.711	0.011	1.705	1.720	80	*4*
C_{ar}—Cl	$\mathbf{C}_{ar}$—**Cl** (mono-Cl + *m,p*-Cl_2)	1.739	1.741	0.010	1.734	1.745	340	*4*
	$\mathbf{C}_{ar}$—**Cl** (*o*-Cl_2)	1.720	1.720	0.010	1.713	1.717	364	*4*
Csp^1—Cl	see HCLENE10 (1.634, 1.646)							
Csp^3—F	Omitting 1,2-difluorides:							
	C—**C**H_2—**F** and C_2—**C**H—**F**	1.399	1.399	0.017	1.389	1.408	25	*4*
	C_3—**C**—**F**	1.428	1.431	0.009	1.421	1.435	11	*4*
	(C*,H)$_2$—**C**—**F**$_2$	1.349	1.347	0.012	1.342	1.356	58	*4*
	C*—**C**—**F**$_3$	1.336	1.334	0.007	1.330	1.344	12	*4*
	F—**C***—**C***—**F**	1.371	1.374	0.007	1.362	1.375	26	*4*
	X_3—**C**—**F** (*X* = C,H,N,O)	1.386	1.389	0.033	1.373	1.408	70	*4*
	X_2—**C**—**F**$_2$ (*X* = C,H,N,O)	1.351	1.349	0.013	1.342	1.356	58	*4*
	X—**C**—**F**$_3$ (*X* = C,H,N,O)	1.322	1.323	0.015	1.314	1.332	309	*4*
	F—**C**(—*X*)$_2$—**C**(—*X*)$_2$—**F** (*X* = C,H,N,O)	1.373	1.374	0.009	1.362	1.377	30	*4*
	F—**C**(—*X*)$_2$—NO_2 (*X* = any substituent)	1.320	1.319	0.009	1.312	1.327	18	
Csp^2—F	C=**C**—**F** (C,H,N,O substituents on C)	1.340	1.340	0.013	1.334	1.346	34	*4*
C_{ar}—F	$\mathbf{C}_{ar}$—**F** (mono-F + *m,p*-F_2)	1.363	1.362	0.008	1.357	1.368	38	*4*
	$\mathbf{C}_{ar}$—**F** (*o*-F_2)	1.340	1.340	0.009	1.336	1.344	167	*4*
Csp^3—H	C—**C**—**H**$_3$ (methyl)	1.059	1.061	0.030	1.039	1.083	83	*21*
	C_2—**C**—**H**$_2$ (primary)	1.092	1.095	0.013	1.088	1.099	100	*21*
	C_3—**C**—**H** (secondary)	1.099	1.097	0.004	1.095	1.103	14	*21*
	$C_{2,3}$—**C**—**H** (primary and secondary)	1.093	1.095	0.012	1.089	1.100	118	*21*
	X—**C**—**H**$_3$ (methyl)	1.066	1.074	0.028	1.049	1.087	160	*21*
	X_2—**C**—**H**$_2$ (primary)	1.092	1.095	0.012	1.088	1.099	230	*21*
	X_3—**C**—**H** (secondary)	1.099	1.099	0.007	1.095	1.103	117	*21*
	$X_{2,3}$—**C**—**H** (primary and secondary)	1.094	1.096	0.011	1.091	1.100	348	*21*
Csp^2—H	C—C=**C**—**H**	1.077	1.079	0.012	1.074	1.085	14	*21*
C_{ar}—H	$\mathbf{C}_{ar}$—**H**	1.083	1.083	0.011	1.080	1.087	218	*21*
Csp^3—I	**C***—**I**	2.162	2.159	0.015	2.149	2.179	15	*4*
C_{ar}—I	$\mathbf{C}_{ar}$—**I**	2.095	2.095	0.015	2.089	2.104	51	*4*
Csp^3—N(4)	**C***—**N**H_3^+	1.488	1.488	0.013	1.482	1.495	298	
	(C*)$_2$—**N**H_2^+	1.494	1.493	0.016	1.484	1.503	249	
	(C*)$_3$—**N**H^+	1.502	1.502	0.015	1.491	1.512	509	
	(C*)$_4$—**N**$^+$	1.510	1.509	0.020	1.496	1.523	319	
	C*—**N**$^+$ (overall)	1.499	1.498	0.018	1.488	1.510	1370	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
Csp^3—N(3)	**C***—**N**$^+$ in N-substituted pyridinium	1.485	1.484	0.009	1.477	1.490	32	
	C*—**N**H$_2$ (Nsp^3: pyramidal)	1.469	1.470	0.010	1.462	1.474	19	*22*
	(**C***)$_2$—**N**H (Nsp^3: pyramidal)	1.469	1.467	0.012	1.461	1.477	152	*5, 22*
	(**C***)$_3$—**N** (Nsp^3: pyramidal)	1.469	1.468	0.014	1.460	1.476	1042	*5, 22*
	C*—**N**sp^3 (overall)	1.469	1.468	0.014	1.460	1.476	1201	
	Csp^3—**N**sp^3 in aziridine	1.472	1.471	0.016	1.464	1.482	134	
	in azetidine	1.484	1.481	0.018	1.472	1.495	21	
	in tetrahydropyrrole	1.475	1.473	0.016	1.464	1.483	66	
	in piperidine	1.473	1.473	0.013	1.460	1.479	240	
	Csp^3—Nsp^2 (N planar) in:							*23*
	acyclic amides **C***—**N**H—C=O	1.454	1.451	0.011	1.446	1.461	78	*14*
	β-lactams **C***—**N**(—*X*)—C=O (*endo*)	1.464	1.465	0.012	1.458	1.475	23	*13*
	γ-lactams **C***—**N**H—C=O (*endo*)	1.457	1.458	0.011	1.449	1.465	20	*13*
	C*—**N**(—C*)—C=O (*endo*)	1.462	1.461	0.010	1.453	1.466	15	*13*
	C*—**N**(—**C***)—C=O (*exo*)	1.458	1.456	0.014	1.448	1.465	15	*13*
	δ-lactams **C***—**N**H—C=O (*endo*)	1.478	1.472	0.016	1.467	1.491	6	*14*
	C*—**N**(—C*)—C=O (*endo*)	1.479	1.476	0.007	1.475	1.482	15	*14*
	C*—**N**(—**C***)—C=O (*exo*)	1.468	1.471	0.009	1.462	1.477	15	*14*
	nitro compounds (1,2-dinitro omitted):							
	C—**C**H$_2$—**N**O$_2$	1.485	1.483	0.020	1.478	1.502	8	
	C$_2$—**C**H—**N**O$_2$	1.509	1.509	0.011	1.502	1.511	12	
	C$_3$—**C**—**N**O$_2$	1.533	1.533	0.013	1.530	1.539	17	
	C$_2$—**C**—(**N**O$_2$)$_2$	1.537	1.536	0.016	1.525	1.550	19	
	1,2-dinitro: **N**O$_2$—**C***—**C***—**N**O$_2$	1.552	1.550	0.023	1.536	1.572	32	
Csp^3—N(2)	**C**$^{\#}$—**N**=N	1.493	1.493	0.020	1.477	1.506	54	
	C*—**N**=C—C$_{ar}$	1.465	1.468	0.011	1.461	1.472	75	
Csp^2—N(3)	C=**C**—**N**H$_2$ Nsp^2 planar	1.336	1.344	0.017	1.317	1.348	10	*23*
	C=**C**—**N**H—C$^{\#}$ Nsp^2 planar	1.339	1.340	0.016	1.327	1.351	17	*23*
	C=**C**—**N**—(C$^{\#}$)$_2$ Nsp^2 planar	1.355	1.358	0.014	1.341	1.363	22	*23*
	Nsp^3 pyramidal	1.416	1.418	0.018	1.397	1.432	18	*22*
	Csp^2—Nsp^2 (N planar) in:							*23*
	acyclic amides **N**H$_2$—**C**=O	1.325	1.323	0.009	1.318	1.331	32	*14*
	acyclic amides C*—**N**H—**C**=O	1.334	1.333	0.011	1.326	1.343	78	*14*
	acyclic amides (C*)$_2$—**N**—**C**=O	1.346	1.342	0.011	1.339	1.356	5	*14*
	β-lactams C*—**N**H—**C**=O	1.385	1.388	0.019	1.374	1.396	23	*13*
	γ-lactams C*—**N**H—**C**=O	1.331	1.331	0.011	1.326	1.337	20	*13*
	γ-lactams C*—**N**(—C*)—**C**=O	1.347	1.344	0.014	1.335	1.359	15	*13*
	δ-lactams C*—**N**H—**C**=O	1.334	1.334	0.006	1.330	1.339	6	*14*
	δ-lactams C*—**N**(—C*)—**C**=O	1.352	1.353	0.010	1.344	1.356	15	*14*
	peptides C$^{\#}$—**N**(—*X*)—**C**(—C$^{\#}$)(=O)	1.333	1.334	0.013	1.326	1.340	380	*24*
	ureas (**N**H$_2$)$_2$—**C**=O	1.334	1.334	0.008	1.329	1.339	48	*25,26*
	ureas (C$^{\#}$—**N**H)$_2$—**C**=O	1.347	1.345	0.010	1.341	1.354	26	*25*
	ureas [(C$^{\#}$)$_n$—**N**]$_2$—**C**=O	1.363	1.359	0.014	1.354	1.370	40	*25, 27*
	thioureas (*X*$_2$**N**)$_2$—**C**=S	1.346	1.343	0.023	1.328	1.361	192	
	imides [C$^{\#}$—**C**(=O)]$_2$—**N**H	1.376	1.377	0.012	1.369	1.383	64	
	[C$^{\#}$—**C**(=O)]$_2$—**N**—C$^{\#}$	1.389	1.383	0.017	1.376	1.404	38	
	[Csp^2—**C**(=O)]$_2$—**N**—C$^{\#}$	1.396	1.396	0.010	1.389	1.403	46	
	[Csp^2—**C**(=O)]$_2$—**N**—Csp^2	1.409	1.406	0.020	1.391	1.419	28	
	guanidinium [**C**—(**N**H$_2$)$_3$]$^+$ (unsubstituted)	1.321	1.320	0.008	1.314	1.327	39	
	(any substituent)	1.328	1.325	0.015	1.317	1.333	140	
	in heterocyclic systems (any substituent):							
	1*H*-pyrrole (N1—C2, N1—C5)	1.372	1.374	0.016	1.363	1.384	58	
	indole (N1—C2)	1.370	1.370	0.012	1.364	1.377	40	
	pyrazole (N1—C5)	1.357	1.359	0.012	1.347	1.365	20	
	imidazole (N1—C2)	1.349	1.349	0.018	1.338	1.358	44	
	imidazole (N1—C5)	1.370	1.370	0.010	1.365	1.377	44	
Csp^2—N(2)	in imidazole (N3—C4)	1.376	1.377	0.011	1.369	1.384	44	
C$_{ar}$—N(4)	**C**$_{ar}$—**N**$^+$(C,H)$_3$	1.465	1.466	0.007	1.461	1.470	23	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	d	m	σ	q_l	q_u	n	Note
C_{ar}—N(3)	**C_{ar}—NH$_2$** (Nsp^2: planar)	1.355	1.360	0.020	1.340	1.372	33	*23*
	(Nsp^3: pyramidal)	1.394	1.396	0.011	1.385	1.403	25	*22*
	(overall)	1.375	1.377	0.025	1.363	1.394	98	*28*
	C_{ar}—NH—C$^{\#}$ (Nsp^2: planar)	1.353	1.353	0.007	1.347	1.359	16	*23*
	(Nsp^3: pyramidal)	1.419	1.423	0.017	1.412	1.432	8	*22*
	(overall)	1.380	1.364	0.032	1.353	1.412	31	*28*
	C_{ar}—N—(C$^{\#}$)$_2$ (Nsp^2: planar)	1.371	1.370	0.016	1.363	1.382	41	*23*
	(Nsp^3: pyramidal)	1.426	1.425	0.011	1.421	1.431	22	*22*
	(overall)	1.390	1.385	0.030	1.366	1.420	69	*28*
	in indole (N1—C7a)	1.372	1.372	0.007	1.367	1.376	40	
	C_{ar}—NO$_2$	1.468	1.469	0.014	1.460	1.476	556	
C_{ar}—N(2)	**C_{ar}—N=N**	1.431	1.435	0.020	1.422	1.442	26	
Csp^2=N(3)	in furoxan ($^+$N2=C3)	1.316	1.316	0.009	1.311	1.324	14	
Csp^2=N(2)	**C_{ar}—C=N—C$^{\#}$**	1.279	1.279	0.008	1.275	1.285	75	
	(C,H)$_2$—C=N—OH in oximes	1.281	1.280	0.013	1.273	1.288	67	
	S—C=N—X	1.302	1.302	0.021	1.285	1.319	36	
	in pyrazole (N2=C3)	1.329	1.331	0.014	1.315	1.339	20	
	in imidazole (C2=N3)	1.313	1.314	0.011	1.307	1.319	44	
	in isoxazole (N2=C3)	1.314	1.315	0.009	1.305	1.320	9	
	in furazan (N2=C3, C4=N5)	1.298	1.299	0.006	1.294	1.303	12	
	in furoxan (C4=N5)	1.304	1.306	0.008	1.300	1.308	14	
C_{ar} ⋯ N(3)	**C⋯N$^+$—H** (pyrimidinium)	1.335	1.334	0.015	1.325	1.342	30	
	C⋯N$^+$—C* (pyrimidinium)	1.346	1.346	0.010	1.340	1.352	64	
	C⋯N$^+$—O$^-$ (pyrimidinium)	1.362	1.359	0.013	1.353	1.369	56	
C_{ar} ⋯ N(2)	**C⋯N** (pyridine)	1.337	1.338	0.012	1.300	1.344	269	
	C⋯N (pyrazine)	1.336	1.335	0.022	1.319	1.347	120	
	C⋯N⋯C (pyrimidine)	1.339	1.338	0.015	1.333	1.342	28	
	N⋯C⋯N (pyrimidine)	1.333	1.335	0.013	1.326	1.337	28	
	C⋯N (pyrimidine) (overall)	1.336	1.337	0.014	1.331	1.339	56	
	in any six-membered N-containing aromatic ring:							
	H—C⋯N⋯C—H	1.334	1.334	0.014	1.327	1.341	146	
	H—C⋯N⋯C—C*	1.339	1.341	0.013	1.336	1.345	38	
	C*—C⋯N⋯C—C*	1.345	1.345	0.008	1.342	1.348	24	
	C⋯N⋯C (overall)	1.336	1.337	0.014	1.329	1.344	204	
Csp^1≡N(2)	***X*—N$^+$≡C$^-$** (isocyanide)	1.144	1.147	0.006	1.140	1.148	6	
Csp^1≡N(1)	**C*—C≡N**	1.136	1.137	0.010	1.131	1.142	140	
	C=C—C≡N in TCNQ	1.144	1.144	0.008	1.139	1.149	284	*19*
	C_{ar}—C≡N	1.138	1.138	0.007	1.133	1.143	31	
	***X*—S—C≡N**	1.144	1.141	0.012	1.138	1.151	10	
	(S—C≡N)$^-$	1.155	1.156	0.012	1.147	1.165	14	
Csp^3—O(2)	in alcohols:							
	CH$_3$—OH	1.413	1.414	0.018	1.395	1.425	17	
	C—CH$_2$—OH	1.426	1.426	0.011	1.420	1.431	75	
	C$_2$—CH—OH	1.432	1.431	0.011	1.425	1.439	266	
	C$_3$—C—OH	1.440	1.440	0.012	1.432	1.449	106	
	C*—OH (overall)	1.432	1.431	0.013	1.424	1.441	464	
	in dialkyl ethers:							*29*
	CH$_3$—O—C*	1.416	1.418	0.016	1.405	1.426	110	
	C—CH$_2$—O—C*	1.426	1.424	0.011	1.418	1.435	34	
	C$_2$—CH—O—C*	1.429	1.430	0.010	1.420	1.437	53	
	C$_3$—C—O—C*	1.452	1.450	0.011	1.445	1.458	39	
	C*—O—C* (overall)	1.426	1.425	0.019	1.414	1.437	236	*5*
	in aryl alkyl ethers:							*29*
	CH$_3$—O—C_{ar}	1.424	1.424	0.012	1.417	1.431	616	
	C—CH$_2$—O—C_{ar}	1.431	1.430	0.013	1.422	1.438	188	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
Csp^2—O(2) (*cont.*)	in aryl alkyl ethers (*cont.*)							
	C_2—**C**H—**O**—C_{ar}	1.447	1.446	0.020	1.435	1.466	58	
	C_3—**C**—**O**—C_{ar}	1.470	1.469	0.018	1.456	1.483	55	
	C*—**O**—C_{ar} (overall)	1.429	1.427	0.018	1.419	1.436	917	
	in alkyl esters of carboxylic acids:							*12, 29*
	CH_3—**O**—C(=O)—C*	1.448	1.449	0.010	1.442	1.455	200	
	C—CH_2—**O**—C(=O)—C*	1.452	1.453	0.009	1.445	1.458	32	
	C_2—**C**H—**O**—C(=O)—C*	1.460	1.460	0.010	1.454	1.465	78	
	C_3—**C**—**O**—C(=O)—C*	1.477	1.475	0.008	1.472	1.484	6	
	C*—**O**—C(=O)—C* (overall)	1.450	1.451	0.014	1.442	1.459	314	
	in alkyl esters of α, β-unsaturated acids:							
	C*—**O**—C(=O)—C=C (overall)	1.453	1.452	0.013	1.444	1.459	112	
	in alkyl esters of benzoic acid							
	C*—**O**—C(=O)—C(phenyl) (overall)	1.454	1.454	0.012	1.446	1.463	219	
	in ring systems:							
	oxirane (epoxide) (any substituent)	1.446	1.446	0.014	1.438	1.456	498	*9*
	oxetane (any substituent)	1.463	1.460	0.015	1.451	1.474	16	
	tetrahydrofuran (C,H substituents)	1.442	1.441	0.017	1.430	1.451	154	
	tetrahydropyran (C,H substituents)	1.441	1.442	0.015	1.431	1.451	22	
	β-lactones: **C***—**O**—C(=O)	1.492	1.494	0.010	1.481	1.501	4	*16*
	γ-lactones: **C***—**O**—C(=O)	1.464	1.464	0.012	1.455	1.473	110	*12*
	δ-lactones: **C***—**O**—C(=O)	1.461	1.464	0.017	1.452	1.473	27	*12*
	O—C—O systems in *gem*-diols, and pyranose and furanose sugars:							*30, 31*
	HO—**C***—**O**H	1.397	1.401	0.012	1.388	1.405	18	
	C_5—**O_5**—**C_1**—**O_1**H in pyranoses:							
	O_1 axial (α): C_5—O_5	1.439	1.440	0.008	1.432	1.445	29	
	O_5—C_1	1.427	1.426	0.012	1.421	1.432	29	
	C_1—O_1	1.403	1.400	0.012	1.391	1.412	29	
	O_1 equatorial (β): C_5—O_5	1.435	1.436	0.008	1.429	1.440	17	
	O_5—C_1	1.430	1.431	0.010	1.424	1.436	17	
	C_1—O_1	1.393	1.393	0.007	1.386	1.399	17	
	$\alpha + \beta$ (overall): C_5—O_5	1.439	1.440	0.008	1.432	1.446	60	
	O_5—C_1	1.430	1.429	0.012	1.421	1.436	60	
	C_1—O_1	1.401	1.399	0.011	1.392	1.407	60	
	C_4—**O_4**—**C_1**—**O_1**H in furanoses:							
	(overall values) C_4—O_4	1.442	1.446	0.012	1.436	1.449	18	
	(overall values) O_4—C_1	1.432	1.432	0.012	1.421	1.443	18	
	(overall values) C_1—O_1	1.404	1.405	0.013	1.397	1.409	18	
	C_5—**O_5**—**C_1**—**O_1**—**C*** in pyranoses:							
	O_1 axial (α): C_5—O_5	1.439	1.438	0.010	1.433	1.446	67	
	O_5—C_1	1.417	1.417	0.009	1.410	1.424	67	
	C_1—O_1	1.409	1.409	0.014	1.401	1.417	67	
	O_1—C*	1.435	1.435	0.013	1.427	1.443	67	
	O_1 equatorial (β): C_5—O_5	1.434	1.435	0.006	1.429	1.439	39	
	O_5—C_1	1.424	1.424	0.008	1.418	1.431	39	
	C_1—O_1	1.390	1.390	0.011	1.381	1.400	39	
	O_1—C*	1.437	1.438	0.013	1.428	1.445	39	
	$\alpha + \beta$ (overall): C_5—O_5	1.436	1.436	0.009	1.431	1.442	126	
	O_5—C_1	1.419	1.419	0.011	1.412	1.426	126	
	C_1—O_1	1.402	1.403	0.016	1.391	1.413	126	
	O_1—C*	1.436	1.436	0.013	1.428	1.445	126	
	C_4—**O_4**—**C_1**—**O_1**—**C*** in furanoses:							
	(overall values) C_4—O_4	1.443	1.445	0.013	1.429	1.453	23	
	(overall values) O_4—C_1	1.421	1.418	0.012	1.413	1.431	23	
	(overall values) C_1—O_1	1.410	1.409	0.014	1.401	1.420	23	
	(overall values) O_1—C*	1.439	1.437	0.014	1.429	1.449	23	
	Miscellaneous:							
	C$^{\#}$—**O**—SiX_3	1.416	1.416	0.017	1.405	1.428	29	
	C*—**O**—SO_2—C	1.465	1.461	0.014	1.454	1.475	33	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	d	m	σ	q_l	q_u	n	Note
Csp^2—O(2) (*cont.*)	in enols: C=**C**—**O**H	1.333	1.331	0.017	1.324	1.342	53	
	in enol esters: C=**C**—**O**—C*	1.354	1.353	0.016	1.341	1.363	40	
	in acids: C*—**C**(=O)—**O**H	1.308	1.311	0.019	1.298	1.320	174	
	C=C—**C**(=O)—**O**H	1.293	1.295	0.019	1.279	1.307	22	
	C_{ar}—**C**(=O)—**O**H	1.305	1.311	0.020	1.291	1.317	75	
	in esters: C*—**C**(=O)—**O**—C*	1.336	1.337	0.014	1.328	1.346	551	*12, 29*
	C=C—**C**(=O)—**O**—C*	1.332	1.331	0.011	1.324	1.339	112	
	C_{ar}—**C**(=O)—**O**—C*	1.337	1.335	0.013	1.329	1.344	219	*12*
	C*—**C**(=O)—**O**—C=C	1.362	1.359	0.018	1.351	1.374	26	
	C*—**C**(=O)—**O**—C=C	1.407	1.405	0.017	1.394	1.420	26	
	C*—**C**(=O)—**O**—C_{ar}	1.360	1.359	0.011	1.355	1.367	40	*12*
	in anhydrides: O=**C**—**O**—**C**=O	1.386	1.386	0.011	1.379	1.393	70	
	in ring systems:							
	furan (O1—C2, O1—C5)	1.368	1.369	0.015	1.359	1.377	125	
	isoxazole (O1—C5)	1.354	1.354	0.010	1.345	1.360	9	
	β-lactones: C*—**C**(=O)—**O**—C*	1.359	1.359	0.013	1.348	1.371	4	*13*
	γ-lactones: C*—**C**(=O)—**O**—C*	1.350	1.349	0.012	1.342	1.359	110	*12*
	δ-lactones: C*—**C**(=O)—**O**—C*	1.339	1.339	0.016	1.332	1.347	27	*12*
C_{ar}—O(2)	in phenols: $\mathbf{C}_{ar}$—**O**H	1.362	1.364	0.015	1.353	1.373	511	
	in aryl alkyl ethers: $\mathbf{C}_{ar}$—**O**—C*	1.370	1.370	0.011	1.363	1.377	920	*29, 32*
	in diaryl ethers: $\mathbf{C}_{ar}$—**O**—$\mathbf{C}_{ar}$	1.384	1.381	0.014	1.375	1.391	132	
	in esters: $\mathbf{C}_{ar}$—**O**—C(=O)—C*	1.401	1.401	0.010	1.394	1.408	40	*12*
Csp^2=O(1)	in aldehydes and ketones:							
	C*—**CH**=**O**	1.192	1.912	0.005	1.188	1.197	7	
	$(C^*)_2$—**C**=**O**	1.210	1.210	0.008	1.206	1.215	474	*5*
	$(C^{\#})_2$—**C**=**O** in cyclobutanones	1.198	1.198	0.007	1.194	1.204	12	
	in cyclopentanones	1.208	1.208	0.007	1.203	1.212	155	
	in cyclohexanones	1.211	1.211	0.009	1.207	1.216	312	
	C=C—**C**=**O**	1.222	1.222	0.010	1.216	1.229	225	
	$(C{=}C)_2$—**C**=**O**	1.233	1.229	0.010	1.226	1.242	28	
	C_{ar}—**C**=**O**	1.221	1.218	0.014	1.212	1.229	85	
	$(C_{ar})_2$—**C**=**O**	1.230	1.226	0.015	1.220	1.238	66	
	C=**O** in benzoquinones	1.222	1.220	0.013	1.211	1.231	86	
	delocalized double bonds in carboxylate anions:							
	H—**C**$\cdots\mathbf{O}_2^-$ (formate)	1.242	1.243	0.012	1.234	1.252	24	
	C*—**C**$\cdots\mathbf{O}_2^-$	1.254	1.253	0.010	1.247	1.261	114	
	C=C—**C**$\cdots\mathbf{O}_2^-$	1.250	1.248	0.017	1.238	1.261	52	
	C_{ar}—**C**$\cdots\mathbf{O}_2^-$	1.255	1.253	0.010	1.249	1.262	22	
	HOOC—**C**$\cdots\mathbf{O}_2^-$ (hydrogen oxalate)	1.243	1.247	0.015	1.232	1.256	26	
	$^-\mathbf{O}_2\cdots$**C**—**C**$\cdots\mathbf{O}_2^-$ (oxalate)	1.251	1.251	0.007	1.248	1.254	18	
	in carboxylic acids (X—COOH):							
	C*—**C**(=**O**)—OH	1.214	1.214	0.019	1.203	1.224	175	
	C=C—**C**(=**O**)—OH	1.229	1.226	0.017	1.218	1.237	22	
	C_{ar}—**C**(=**O**)—OH	1.226	1.223	0.020	1.211	1.241	75	
	in esters:							
	C*—**C**(=**O**)—O—C*	1.196	1.196	0.010	1.190	1.202	551	*12*
	C=C—**C**(=**O**)—O—C*	1.199	1.198	0.009	1.193	1.203	113	
	C_{ar}—**C**(=**O**)—O—C*	1.202	1.201	0.009	1.196	1.207	218	*12*
	C*—**C**(=**O**)—O—C=C	1.190	1.190	0.014	1.184	1.198	26	
	C*—**C**(=**O**)—O—C_{ar}	1.187	1.188	0.011	1.181	1.195	40	*12*
	in anhydrides: **O**=**C**—O—**C**=**O**	1.187	1.187	0.010	1.184	1.193	70	
	in β-lactones: C*—**C**(=**O**)—O—C*	1.193	1.193	0.006	1.187	1.198	4	*13*
	γ-lactones: C*—**C**(=**O**)—O—C*	1.201	1.202	0.009	1.196	1.206	109	*12*
	δ-lactones: C*—**C**(=**O**)—O—C*	1.205	1.207	0.008	1.201	1.209	27	*12*
	in amides:							
	NH_2—**C**(—C*)=**O**	1.234	1.233	0.012	1.225	1.243	32	*14*
	(C*—)(C*,H—)N—**C**(—C*)=**O**	1.231	1.231	0.012	1.224	1.238	378	*14*
	β-lactams: C*—NH—**C**=**O**	1.198	1.200	0.012	1.193	1.204	23	*13*

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
Csp^2═O(1) (*cont.*)	in amides (*cont.*)							
	γ-lactams: C*—NH—**C═O**	1.235	1.235	0.008	1.232	1.240	20	*13*
	γ-lactams: C*—N(—C*)—**C═O**	1.225	1.226	0.011	1.217	1.233	15	*13*
	δ-lactams: C*—NH—**C═O**	1.240	1.241	0.003	1.237	1.243	6	*14*
	δ-lactams: O*—N(—C*)—**C═O**	1.233	1.233	0.007	1.229	1.239	15	*14*
	in ureas:							
	$(NH_2)_2$—**C═O**	1.256	1.256	0.007	1.249	1.261	24	*25, 26*
	$(C^{\#}—NH)_2$—**C═O**	1.241	1.237	0.011	1.235	1.245	13	*25*
	$[(C^{\#})_n—N]_2$—**C═O**	1.230	1.230	0.007	1.224	1.234	20	*25, 27*
Csp^3—P(4)	C_3—**P^+**—**C***	1.800	1.802	0.015	1.790	1.812	35	*33*
	C_2—**P**(═O)—**CH_3**	1.791	1.790	0.006	1786	1.795	10	
	C_2—**P**(═O)—**CH_2**—C	1.806	1.806	0.009	1.801	1.813	45	
	C_2—**P**(═O)—**CH**—C_2	1.821	1.821	0.009	1.815	1.828	15	
	C_2—**P**(═O)—**C**—C_3	1.841	1.842	0.008	1.835	1.847	14	
	C_2—**P**(═O)—**C*** (overall)	1.813	1.811	0.017	1.800	1.822	84	
Csp^3—P(3)	C_2—**P**—**C***	1.855	1.857	0.019	1.840	1.870	23	
C_{ar}—P(4)	C_3—**P^+**—**C_{ar}**	1.793	1.792	0.011	1.786	1.800	276	
	C_2—**P**(═O)—**C_{ar}**	1.801	1.802	0.011	1.796	1.807	98	
	Ph_3—**P**═N^+═**P**—**Ph_3**	1.795	1.795	0.008	1.789	1.800	197	
C_{ar}—P(3)	C_2—**P**—**C_{ar}**	1.836	1.837	0.010	1.830	1.844	102	
	$(N⋯)_2$**P**—**C_{ar}** (P⋯N aromatic)	1.795	1.793	0.011	1.788	1.803	43	
Csp^3—S(4)	**C***—**SO_2**—C (C* = CH_3 excluded)	1.786	1.782	0.018	1.774	1.797	75	
	C*—**SO_2**—C (overall)	1.779	1.778	0.020	1.764	1.790	94	
	C*—**SO_2**—O—*X*	1.745	1.744	0.009	1.738	1.754	7	*34*
	C*—**SO_2**—N—X_2	1.758	1.736	0.018	1.746	1.773	17	*34*
Csp^3—S(3)	**C***—**S**(═O)—C (C* = CH_3 excluded)	1.818	1.814	0.024	1.802	1.829	69	
	C*—**S**(═O)—C (overall)	1.809	1.806	0.025	1.793	1.820	88	
	CH_3—**S^+**—X_2	1.786	1.787	0.007	1.779	1.792	21	
	C*—**S^+**—X_2 (C* = CH_3 excluded)	1.823	1.820	0.016	1.812	1.834	18	
	C*—**S^+**—C_2 (overall)	1.804	1.794	0.025	1.788	1.820	41	
Csp^3—S(2)	**C***—**SH**	1.808	1.805	0.010	1.800	1.819	6	
	CH_3—**S**—C*	1.789	1.787	0.008	1.784	1.794	9	
	C—**CH_2**—**S**—C*	1.817	1.816	0.013	1.808	1.824	92	
	C_2—**CH**—**S**—C*	1.819	1.819	0.011	1.811	1.825	32	
	C_3—**C**—**S**—C*	1.856	1.860	0.011	1.854	1.863	26	
	C*—**S**—**C*** (overall)	1.819	1.817	0.019	1.809	1.827	242	
	in thiirane	1.834	1.835	0.025	1.810	1.858	4	*9*
	in thietane: see ZCMXSP (1.817, 1.844)							
	in tetrahydrothiophene	1.827	1.826	0.018	1.811	1.837	20	
	in tetrahydrothiopyran	1.823	1.821	0.014	1.812	1.832	24	
	C—**CH_2**—**S**—S—*X*	1.823	1.820	0.014	1.813	1.832	41	
	C_3—**C**—**S**—S—*X*	1.863	1.865	0.015	1.848	1.878	11	
	C*—**S**—S—*X* (overall)	1.833	1.828	0.022	1.818	1.848	59	
Csp^2—S(2)	C═**C**—**S**—C*	1.751	1.755	0.017	1.740	1.764	61	
	C═**C**—**S**—C═C (in tetrathiafulvalene)	1.741	1.741	0.011	1.733	1.750	88	
	C═**C**—**S**—C═C (in thiophene)	1.712	1.712	0.013	1.703	1.722	60	
	O═**C**—**S**—$C^{\#}$	1.762	1.759	0.018	1.747	1.778	20	
C_{ar}—S(4)	**C_{ar}**—**SO_2**—C	1.763	1.764	0.009	1.756	1.769	96	
	C_{ar}—**SO_2**—O—*X*	1.752	1.750	0.008	1.749	1.756	27	
	C_{ar}—**SO_2**—N—X_2	1.758	1.759	0.013	1.749	1.765	106	*35*
C_{ar}—S(3)	**C_{ar}**—**S**(═O)—C	1.790	1.790	0.010	1.783	1.798	41	
	C_{ar}—**S^+**—X_2	1.778	1.779	0.010	1.771	1.787	10	
C_{ar}—S(2)	**C_{ar}**—**S**—C*	1.773	1.774	0.009	1.765	1.779	44	
	C_{ar}—**S**—**C_{ar}**	1.768	1.767	0.010	1.762	1.774	158	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
C_{ar}—S(2) (*cont.*)	$\mathbf{C}_{ar}$—**S**—$\mathbf{C}_{ar}$ (in phenothiazine) $\mathbf{C}_{ar}$—**S**—S—*X*	1.764 1.777	1.764 1.777	0.008 0.012	1.760 1.767	1.769 1.785	48 47	
C*sp*^{1}—S(2)	N≡**C**—**S**—*X*	1.679	1.683	0.026	1.645	1.698	10	
C*sp*^{1}—S(1)	(N≡**C**—**S**)$^-$	1.630	1.630	0.014	1.619	1.641	14	
C*sp*^{2}=S(1)	$(C^*)_2$—**C**=**S**: see IPMUDS (1.599) $(C_{ar})_2$—**C**=**S**: see CELDOM (1.611) $(X)_2$—**C**=**S** (*X* = C,N,O,S) X_2N—**C**(=**S**)—S—*X* $(X_2N)_2$—**C**=**S** (thioureas) N—**C**(⋯**S**)$_2$	 1.671 1.660 1.681 1.720	 1.675 1.660 1.684 1.721	 0.024 0.016 0.020 0.012	 1.656 1.648 1.669 1.709	 1.689 1.674 1.693 1.731	 245 38 96 20	
C*sp*^{3}—Se	$\mathbf{C}^{\#}$—**Se**	1.970	1.967	0.032	1.948	1.998	21	
C*sp*^{2}—Se(2)	C=**C**—**Se**—**C**=C (in tetraselenafulvalene)	1.893	1.895	0.013	1.882	1.902	32	
C_{ar}—Se(3)	$\mathbf{Ph}_3$—$\mathbf{Se}^+$	1.930	1.929	0.006	1.924	1.936	13	
C*sp*^{3}—Si(5)	$\mathbf{C}^{\#}$—$\mathbf{Si}^-$—X_4	1.874	1.876	0.015	1.859	1.884	9	
C*sp*^{3}—Si(4)	$\mathbf{C}H_3$—**Si**—X_3 **C***—**Si**—X_3 (C* = CH_3 excluded) **C***—**Si**—X_2 (overall)	1.857 1.888 1.863	1.857 1.887 1.861	0.018 0.023 0.024	1.848 1.872 1.850	1.869 1.905 1.875	552 124 681	
C_{ar}—Si(4)	$\mathbf{C}_{ar}$—**Si**—X_3	1.868	1.868	0.014	1.857	1.878	178	
C*sp*^{1}—Si(4)	C≡**C**—**Si**—X_3	1.837	1.840	0.012	1.824	1.849	8	
C*sp*^{3}—Te	$\mathbf{C}^{\#}$—**Te**	2.158	2.159	0.030	2.128	2.177	13	
C_{ar}—Te	$\mathbf{C}_{ar}$—**Te**	2.116	2.115	0.020	2.104	2.130	72	
C*sp*^{2}=Te	see CEDCUJ (2.044)							
Cl—Cl	see PHASCL (2.306, 2.227)							
Cl—I	see CMBIDZ (2.563), HXPASC (2.541, 2.513), METAMM (2.552), BQUINI (2.416, 2.718)							
Cl—N	see BECTAE (1.743–1.757), BOGPOC (1.705)							
Cl—O(1)	in ClO_4^-	1.414	1.419	0.026	1.403	1.431	252	
Cl—P	(N⋯)$_2$**P**—**Cl** (N⋯P aromatic) **Cl**—**P** (overall)	1.997 2.008	1.994 2.001	0.015 0.035	1.989 1.986	2.004 2.028	46 111	
Cl—S	**Cl**—**S** (overall) see also longer bonds in CILSAR (2.283), BIHXIZ (2.357), CANLUY (2.749)	2.072	1.079	0.023	2.047	2.091	6	
Cl—Se	See BIRGUE10, BIRHAL10, CTCNSE (2.234–2.851)							
Cl—Si(4)	**Cl**—**Si**—X_3 (monochloro) $\mathbf{Cl}_2$—**Si**—X_2 and $\mathbf{Cl}_3$—**Si**—*X*	2.072 2.020	2.075 2.012	0.009 0.015	2.066 2.007	2.078 2.036	5 5	
Cl—Te	Cl—Te in range 2.34–2.60 see also longer bonds in BARRIV, BOJPUL, CETUTE, EPHTEA, OPNTEC10 (2.73–2.94)	2.520	2.515	0.034	2.493	2.537	22	*36*
F—N(3)	**F**—**N**—C_2 and $\mathbf{F}_2$—**N**—C	1.406	1.404	0.016	1.395	1.416	9	
F—P(6)	in hexafluorophosphate, PF_6^-	1.579	1.587	0.025	1.563	1.598	72	
P—P(3)	(N⋯)$_2$**P**—**F** (N⋯P aromatic)	1.495	1.497	0.016	1.481	1.510	10	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
F—S	43 observations in range 1.409–1.770 in a wide variety of environments							
	F—**S**(6) in $\mathbf{F_2}$—$\mathbf{SO_2}$—C_2 (see FPSULF10, BETJOZ)	1.640	1.646	0.011	1.626	1.649	6	
	F—**S**(4) in $\mathbf{F_2}$—**S**(=O)—N (see BUDTEZ)	1.527	1.528	0.004	1.524	1.530	24	*37*
F—Si(6)	in SiF_6^{2-}	1.694	1.701	0.013	1.677	1.703	6	
F—Si(5)	**F**—$\mathbf{Si}^-$—X_4	1.636	1.639	0.035	1.602	1.657	10	
F—Si(4)	**F**—**Si**—X_3	1.588	1.587	0.014	1.581	1.599	24	
F—Te	see CUCPIZ [F—Te(6) = 1.942, 1.937], FPHTEL [F—Te(4) = 2.006]							
H—N(4)	X_3—$\mathbf{N}^+$—**H**	1.033	1.036	0.022	1.026	1.045	87	*21*
H—N(3)	X_2—**N**—**H**	1.009	1.010	0.019	0.997	1.023	95	*21*
H—O(2)	in alcohols C*—**O**—**H**	0.967	0.969	0.010	0.959	0.974	63	*21*
	$C^{\#}$—**O**—**H**	0.967	0.970	0.010	0.959	0.974	73	*21*
	in acids O=C—**O**—**H**	1.015	1.017	0.017	1.001	1.031	16	*21, 38*
I—I	in I_3^-	2.917	2.918	0.011	2.907	2.927	6	
I—N	see BZPRIB, CMBIDZ, HMTITI, HMTNTI, IFORAM, IODMAM (2.042–2.475)							
I—O	X—**I**—**O** (see BZPRIB, CAJMAB, IBZDAC11)	2.144	2.144	0.028	2.127	2.164	6	
	for IO_6^- see BOVMEE (1.829–1.912)							
I—P(3)	see CEHKAB (2.490–2.493)							†
I—S	see DTHIBR10 (2.687), ISUREA10 (2.629), BZTPPI (3.251)							
I—Te(4)	**I**—**Te**—X_3	2.926	2.928	0.026	2.902	2.944	8	
N(4)—N(3)	X_3—$\mathbf{N}^+$—$\mathbf{N}^0$—X_2 (N^0 planar)	1.414	1.414	0.005	1.412	1.418	13	
N(3)—N(3)	(C)(C,H)—$\mathbf{N}_a$—$\mathbf{N}_b$—(C)(C,H)							*5, 39*
	N_a, N_b pyramidal	1.454	1.452	0.021	1.444	1.457	44	*40*
	N_a pyramidal, N_b planar	1.420	1.420	0.015	1.407	1.433	68	*40*
	N_a, N_b planar	1.401	1.401	0.018	1.384	1.418	40	*40*
	overall	1.425	1.425	0.027	1.407	1.443	139	
N(3)—N(2)	in pyrazole (**N**1—**N**2)	1.366	1.366	0.019	1.350	1.375	20	
	in pyridazinium ($\mathbf{N1}^+$···**N**2)	1.350	1.349	0.010	1.345	1.361	7	
N(2)···N(2)	**N**···**N** (aromatic) in pyridazine							
	with C,H as *ortho* substituents	1.304	1.300	0.019	1.287	1.326	6	
	with N,Cl as *ortho* substituents	1.368	1.373	0.011	1.362	1.375	9	
N(2)=N(2)	$C^{\#}$—**N**=**N**—$C^{\#}$ (*cis*)	1.245	1.244	0.009	1.239	1.252	21	
	(*trans*)	1.222	1.222	0.006	1.218	1.227	6	
	(overall)	1.240	1.241	0.012	1.230	1.251	27	
	C_{ar}—**N**=**N**—C_{ar}	1.255	1.253	0.016	1.247	1.262	13	
	X—**N**=**N**=N (azides)	1.216	1.226	0.028	1.202	1.237	19	
N(2)=N(1)	X—N=**N**=**N** (azides)	1.124	1.128	0.015	1.114	1.137	19	
N(3)—O(2)	$(C,H)_2$—**N**—**O**H (Nsp^2: planar)	1.396	1.394	0.012	1.390	1.401	28	
	C_2—**N**—**O**—C (Nsp^3: pyramidal)	1.463	1.465	0.012	1.457	1.468	22	
	C_2—**N**—**O**—C (Nsp^2: planar)	1.397	1.394	0.011	1.388	1.409	12	
	in furoxan (N2—O1)	1.438	1.436	0.009	1.430	1.447	14	
N(3)—O(1)	$(C···)_2\mathbf{N}^+$—$\mathbf{O}^-$ in pyridine *N*-oxides	1.304	1.299	0.015	1.291	1.316	11	
	in furoxan ($^+$N2—O6$^-$)	1.234	1.234	0.008	1.228	1.240	14	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
N(2)—O(2)	in oximes:							
	$(C^{\#})_2$—C═**N**—**O**H	1.416	1.418	0.006	1.416	1.420	7	
	(H)(Csp^2)—C═**N**—**O**H	1.390	1.390	0.011	1.380	1.401	20	
	($C^{\#}$)(Csp^2)—C═**N**—**O**H	1.402	1.403	0.010	1.393	1.410	18	
	(Csp^2)$_2$—C═**N**—**O**H	1.378	1.377	0.017	1.365	1.393	16	
	$(C,H)_2$—C═**N**—**O**H (overall)	1.394	1.395	0.018	1.379	1.408	67	
	in furazan (O1—N2, O1—N5)	1.385	1.383	0.013	1.378	1.392	12	
	in furoxan (O1—N5)	1.380	1.380	0.011	1.370	1.388	14	
	in isoxazole (O1—N2)	1.425	1.425	0.010	1.417	1.434	9	
N(3)═O(1)	in nitrate ions $\mathbf{NO_3^-}$	1.239	1.240	0.020	1.227	1.251	105	
	in nitro groups:							
	C*—$\mathbf{NO_2}$	1.212	1.214	0.012	1.206	1.221	84	
	$C^{\#}$—$\mathbf{NO_2}$	1.210	1.210	0.011	1.203	1.218	251	
	C_{ar}—$\mathbf{NO_2}$	1.217	1.218	0.011	1.211	1.215	1116	
	C—$\mathbf{NO_2}$ (overall)	1.218	1.219	0.013	1.210	1.226	1733	
N(3)—P(4)	X_2—**P**(═*X*)—**N**X_2 Nsp^2: planar	1.652	1.651	0.024	1.634	1.670	205	
	Nsp^3: pyramidal	1.683	1.683	0.005	1.680	1.686	6	
	(overall)	1.662	1.662	0.029	1.639	1.682	358	
	subsets of this group are:							
	O_2—**P**(═S)—**N**X_2	1.628	1.624	0.015	1.615	1.634	9	
	C—**P**(═S)—$(\mathbf{N}X_2)_2$	1.691	1.694	0.018	1.678	1.703	28	
	O—**P**(═S)—$(\mathbf{N}X_2)_2$	1.652	1.654	0.014	1.642	1.664	28	
	P(═O)—$(\mathbf{N}X_2)_3$	1.663	1.668	0.026	1.640	1.679	78	
N(3)—P(3)	—**N***X*—**P**(—*X*)—**N***X*—**P**(—*X*)— (P_2N_2 ring)	1.730	1.721	0.017	1.716	1.748	20	
	—**N***X*—**P**(═S)—**N***X*—**P**(═S)— (P_2N_2 ring)	1.697	1.697	0.015	1.690	1.703	44	
	in P-substituted phosphazenes:							
	$(N\equiv)_2$**P**—**N** (amino)	1.637	1.638	0.014	1.625	1.651	16	
	(aziridinyl)	1.672	1.674	0.010	1.665	1.676	15	
N(2)═P(4)	Ph_3—**P**═$\mathbf{N^+}$═**P**—Ph_3	1.571	1.573	0.013	1.563	1.580	66	
	Ph_3—**P**═**N**—C,S	1.599	1.597	0.018	1.580	1.615	7	
N(2)⋮P(3)	**N**⋮**P** aromatic in phosphazenes	1.582	1.582	0.019	1.571	1.594	126	
	in **P**⋮**N**⋮S	1.604	1.606	0.009	1.594	1.612	36	
N(3)—S(4)	C—$\mathbf{SO_2}$—$\mathbf{NH_2}$	1.600	1.601	0.012	1.591	1.610	14	*35*
	C—$\mathbf{SO_2}$—**N**H—$C^{\#}$	1.633	1.633	0.019	1.615	1.652	47	*35*
	C—$\mathbf{SO_2}$—**N**—$(C^{\#})_2$	1.642	1.641	0.024	1.623	1.659	38	*35*
N(3)—S(2)	C—**S**—**N**X_2 Nsp^2: planar	1.710	1.707	0.019	1.698	1.722	22	*23*
	(for Nsp^3 pyramidal see MODIAZ: 1.765)							
	X—**S**—**N**X_2 Nsp^2: planar	1.707	1.705	0.012	1.699	1.715	30	*23*
N(2)—S(2)	C═**N**—**S**—*X*	1.656	1.663	0.027	1.632	1.677	36	
N(2)⋮S(2)	**N**⋮**S** aromatic in P⋮**N**⋮**S**	1.560	1.558	0.011	1.554	1.563	37	
N(2)═S(2)	**N**═**S** in **N**═**S**═**N** and **N**═**S**═S	1.541	1.546	0.022	1.521	1.558	37	
N(3)—Se	see COJCUZ (1.830), DSEMOR10 (1.846, 1.852), MORTRS10 (1.841)							
N(2)—Se	see SEBZQI (1.805), NAPSEZ10 (1.809, 1.820)							
N(2)═Se	see CISMUM (1.790, 1.791)							
N(3)—Si(5)	see DMESIP01, BOJLER, CASSAQ, CASYOK, CECXEN, CINTEY, CIPBUY, FMESIB, MNPSIL, PNPOSI (1.973–2.344)							
N(3)—Si(4)	X_3—**Si**—**N**X_2 (overall)	1.748	1.746	0.022	1.735	1.757	170	
	subsets of this group are:							
	X_3—**Si**—**N**H*X*	1.714	1.719	0.014	1.702	1.727	16	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	*d*	*m*	σ	q_l	q_u	*n*	Note
N(3)—Si(4) (*cont.*)	X_3—**Si**—**N**X—**Si**—X_3 acyclic	1.743	1.744	0.016	1.731	1.755	45	
	N—**Si**—**N** in four-membered rings	1.742	1.742	0.009	1.735	1.748	53	
	N—**Si**—**N** in five-membered rings	1.741	1.742	0.019	1.726	1.749	33	
N(2)—Si(4)	X_3—**Si**—**N**$^-$—**Si**—X_3	1.711	1.712	0.019	1.693	1.729	15	
N—Te	see ACLTEP (2.402), BIBLAZ (1.980), CESSAU (2.023)							
O(2)—O(2)	C*—**O**—**O**—C*,H τ(OO) = 70–85°	1.464	1.464	0.009	1.458	1.472	12	
	τ(OO) approx. 180°	1.482	1.480	0.005	1.478	1.486	5	
	(overall)	1.469	1.471	0.012	1.461	1.478	17	
	O=C—**O**—**O**—C=O see ACBZPO01 (1.446), CEYLUN (1.452), CIMHIP (1.454)							
	Si—**O**—**O**—Si	1.496	1.499	0.005	1.490	1.499	10	
O(2)—P(5)	X—**P**—(**O**X)$_4$							*41*
	trigonal bipyramidal: axial	1.689	1.685	0.024	1.675	1.712	20	
	equatorial	1.619	1.622	0.024	1.604	1.628	20	
	square pyramidal	1.662	1.661	0.020	1.649	1.673	28	
O(2)—P(4)	C—**O**—**P**(⋯O)$_3^{2-}$	1.621	1.622	0.007	1.615	1.628	12	
	(H—**O**)$_2$—**P**(⋯O)$_2^-$	1.560	1.561	0.009	1.555	1.566	16	
	(C—**O**)$_2$—**P**(⋯O)$_2^-$	1.608	1.607	0.013	1.599	1.615	16	
	(C$^{\#}$—**O**)$_3$—**P**=O	1.558	1.554	0.011	1.550	1.564	30	
	(C$_{ar}$—**O**)$_3$—**P**=O	1.587	1.588	0.014	1.572	1.599	19	
	X—**O**—**P**(=O)—(C,N)$_2$	1.590	1.585	0.016	1.577	1.601	33	
	(X—**O**)$_2$—**P**(=O)—(C,N)	1.571	1.572	0.013	1.563	1.579	70	
O(2)—P(3)	(N⋯)$_2$**P**—**O**—C (N⋯P aromatic)	1.573	1.573	0.011	1.563	1.584	16	
O(1)=P(4)	C—O—**P**(⋯**O**)$_3^{2-}$ (delocalized)	1.513	1.512	0.008	1.508	1.518	42	
	(H—O)$_2$—**P**(⋯**O**)$_2^-$ (delocalized)	1.503	1.503	0.005	1.499	1.508	16	
	(C—O)$_2$—**P**(⋯**O**)$_2^-$ (delocalized)	1.483	1.485	0.008	1.474	1.490	16	
	(C—O)$_3$—**P**=**O**	1.449	1.448	0.007	1.446	1.452	18	
	C$_3$—**P**=**O**	1.489	1.486	0.010	1.481	1.496	72	
	N$_3$—**P**=**O**	1.461	1.462	0.014	1.449	1.470	26	
	(C)$_2$(N)—**P**=**O**	1.487	1.489	0.007	1.479	1.493	5	
	(C,N)$_2$(O)—**P**=**O**	1.467	1.465	0.007	1.462	1.472	33	
	(C,N)(O)$_2$—**P**=**O**	1.457	1.458	0.009	1.454	1.462	35	
O(2)—S(4)	C—**O**—**S**O$_2$—C	1.577	1.576	0.015	1.566	1.584	41	
	C—**O**—**S**O$_2$—CH$_3$	1.569	1.569	0.013	1.556	1.582	7	
	C—**O**—**S**O$_2$—C$_{ar}$	1.580	1.578	0.015	1.571	1.588	27	
O(1)=S(4)	C—**S**O$_2$—C	1.436	1.437	0.010	1.431	1.442	316	*42*
	X—**S**O$_2$—NX_2	1.428	1.428	0.010	1.422	1.434	326	
	C—**S**O$_2$—N—(C,H)$_2$	1.430	1.430	0.009	1.425	1.435	206	
	C—**S**O$_2$—O—C	1.423	1.423	0.008	1.418	1.428	82	
	in **S**O$_4^{2-}$	1.472	1.473	0.013	1.463	1.481	104	
O(1)=S(3)	C—**S**(=**O**)—C	1.497	1.498	0.013	1.489	1.505	90	*5*
O—Se	see BAPPAJ, BIRGUE10, BIRHAL10, CXMSEO, DGLYSE, SPSEBU (1.597 for O=Se to 1.974 for O—Se)							
O(2)—Si(5)	(X—**O**)$_3$—**Si**—(N)(C)	1.663	1.658	0.023	1.650	1.665	21	
O(2)—Si(4)	X_3—**Si**—**O**—X (overall)	1.631	1.630	0.022	1.617	1.646	191	
	subsets of this group are:							
	X_3—**Si**—**O**—C$^{\#}$	1.645	1.647	0.012	1.634	1.652	29	
	X_3—**Si**—**O**—Si—X_3	1.622	1.625	0.014	1.614	1.631	70	
	X_3—**Si**—**O**—**O**—**Si**—X_3	1.680	1.676	0.008	1.673	1.688	10	
O(2)—Te(6)	(X—**O**)$_6$—**Te**	1.927	1.927	0.020	1.908	1.942	16	
O(2)—Te(4)	(X—**O**)$_2$—**Te**—X_2	2.133	2.136	0.054	2.078	2.177	12	

Table 9.5.1.1. *Average lengths (cont.)*

Bond	Substructure	d	m	σ	q_l	q_u	n	Note
P(4)—P(4)	X_3—**P**—**P**—X_3	2.256	2.259	0.025	2.243	2.277	6	
P(4)—P(3)	see CECHEX (2.197), COZPIQ (2.249)							
P(3)—P(3)	X_2—**P**—**P**—X_2	2.214	2.210	0.022	2.200	2.224	41	
P(4)═P(4)	see BUTSUE (2.054)							
P(3)═P(3)	see BALXOB (2.034)							
P(4)═S(1)	C_3—**P**═**S** $(N,O)_2(C)$—**P**═**S** $(N,O)_3$—**P**═**S**	1.954 1.922 1.913	1.952 1.924 1.914	0.005 0.014 0.014	1.950 1.913 1.906	1.957 1.927 1.921	13 26 50	
P(4)═Se(1)	X_3—**P**═**Se**	2.093	2.099	0.019	2.075	2.108	12	
P(3)—Si(4)	X_2—**P**—**Si**—X_3: 3- and 4-rings excluded (see BOPFER, BOPFIV, CASTOF10, COZVIW: 2.201–2.317)	2.264	2.260	0.019	2.249	2.283	22	
P(4)═Te(1)	see MOPHTE (2.356), TTEBPZ (2.327)							
S(2)—S(2)	C—**S**—**S**—C τ (SS) = 75–105° τ (SS) = 0–20° (overall) in polysulfide chain —**S**—**S**—**S**—	2.031 2.070 2.048 2.051	2.029 2.068 2.045 2.050	0.015 0.022 0.026 0.022	2.021 2.057 2.028 2.037	2.038 2.077 2.068 2.065	46 28 99 126	
S(2)—S(1)	X—N═**S**—**S**	1.897	1.896	0.012	1.887	1.908	5	
S—Se(4)	see BUWZUO (2.264, 2.269)							
S—Se(2)	X—**Se**—**S** (any)	2.193	2.195	0.015	2.174	2.207	9	
S(2)—Si(4)	X_3—**Si**—**S**—X	2.145	2.138	0.020	2.130	2.158	19	
S(2)—Te	X—**S**—**Te** (any) X═**S**—**Te** (any)	2.405 2.682	2.406 2.686	0.022 0.035	2.383 2.673	2.424 2.694	10 28	
Se(2)—Se(2)	X—**Se**—**Se**—X	2.340	2.340	0.024	2.315	2.361	15	
Se(2)—Te(2)	see BAWFUA, BAWGAH (2.524–2.561)							†
Si(4)—Si(4)	X_3—**Si**—**Si**—X_3 three-membered rings excluded: see CIHRAM (2.511)	2.359	2.359	0.012	2.349	2.366	42	
Te—Te	see CAHJOK (2.751, 2.704)							

† See opening paragraph of Section 9.5.3. For numbered footnotes, see Appendix 1.

references