

**List of CSD REFCODES with compound names and references**

ACURID:  $\beta$ -5-Acetyl-2'-deoxyuridine. Barr, P. J.; Chananont, P.; Hamor, T. A.; Jones, A. S.; O'Leary, M. K.; Walker, R. T. The Synthesis and Crystal-Structure of 5-Acetyl-2'-Deoxyuridine. *Tetrahedron* **1980**, *36*, 1269-1273.

ADOSHC: Adenosine hydrochloride. Shikata, K.; Ueki, T.; Mitsui, T. Crystal and Molecular Structure of Adenosine Hydrochloride. *Acta Crystallogr.* **1973**, *B29*, 31-38.

ADENOS01: Adenosine. Klooster, W. T.; Ruble, J. R.; Craven, B. M.; McMullan, R. K. Structure and Thermal Vibrations of Adenosine from Neutron Diffraction Data at 123 K. *Acta Crystallogr.* **1991**, *B47*, 376-383.

BENZEN06: Hexadeutero-benzene. Jeffrey, G. A.; Ruble, J. R.; McMullan, R. K.; Pople, J. A. The Crystal Structure of Deuterated Benzene. *Proc. R. Soc. London* **1987**, *A414*, 47-57.

BEURID10: Uridine. Green, E. A.; Rosenstein, R. D.; Shiono, R.; Abraham, D. J.; Trus, B. L.; Marsh, R. E. Crystal Structure of Uridine. *Acta Crystallogr.* **1975**, *B31*, 102-107.

BIMFIM10:  $N^{1,6}$ -Ethenoadenosine hydrochloride. Jaskolski, M. Crystal and Molecular Structure of  $N^{1,6}$ -Ethenoadenosine Hydrochloride. *J. Cryst. Spectrosc. Res.* **1984**, *14*, 45-47.

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CALBOG: 1,1,3-Trichloroindene. Linden, A.; Guspanova, J.; Hansen, H.-J. *Private Communication*, 1998.

CEFJUS: *O*<sup>4</sup>-Methyluridine. Brennan, R. G.; Prive, G. G.; Blonski, W. J. P.; Hruska, F. E.; Sundaralingam, M. Molecular and Crystal-Structure of *O*<sup>4</sup>-Methyluridine – Reaction Coordinates for an Incipient Nucleophilic-Attack Seen By Short Intermolecular Sugar Base Interactions. *J. Am. Chem. Soc.* **1983**, *105*, 7737-7742.

CLPRCV: *catena-bis*( $\mu^2$ -Chloro)-tetrachloro-purinium-di-copper(II). Sheldrick, W. S. Poly-Di- $\mu$ -Chloro-Tetrachloro(Purinium)Dicopper(II). *Acta Crystallogr.* **1981**, *B37*, 945-946.

CUTVAO: Xanthosine. Lesyng, B.; Marck, C.; Saenger, W. Z. The Crystal-Structure of Anhydrous Xanthosine Displays Intramolecular O(2')H<sup>+</sup> O(3') Hydrogen-Bond. *Naturforsch.* **1984**, *C39*, 720-724.

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DAZCYT10: 3-Deazacytidine. Hutcheon, W. L. B.; James, M. N. G. Crystal Structure of 3-Deazacytidine. *Acta Crystallogr.* **1977**, *B33*, 2224-2228.

DEFPOT: *N*<sup>6</sup>-Methyl-2'-deoxyadenosine. Sato, T. Structure of *N*<sup>6</sup>-methyl-2'-deoxyadenosine *Acta Crystallogr.* **1985**, *C41*, 1624-1625.

DEHQOW: 1-Deaza-adenosine monohydrate. Seela, F.; Debelak, H.; Reuter, H.; Kastner, G.; Mikhailopulo, I. A. Different Conformations of 1-Deazaadenosine and its 2'-Deoxyribonucleoside in the Solid State and in Solution. *Tetrahedron* **1999**, *55*, 1295-1308.

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DOXPOV: *O*<sup>4</sup>-Methylthymidine. Brennan, R. G.; Pyzalska, D.; Blonski, W. J. P.; Hruska, F. E.; Sundaralingam, M. Crystal Structure of the Promutagen *O*<sup>4</sup>-Methylthymidine - Importance of the Anti Conformation of the *O*<sup>(4)</sup> Methoxy Group and Possible Mispairing of *O*<sup>4</sup>-Methylthymidine with Guanine. *Biochemistry*, **1986**, *25*, 1181-1185.

ETCYTC: 3,*N*<sup>4</sup>-Ethenocytidine hydrochloride. Wang, A. H.-J.; Barrio, J. R.; Paul, I. C. Crystal and Molecular Structure of 3,*N*<sup>4</sup>-Ethenocytidine Hydrochloride - Study of Dimensions and Molecular Interactions of Fluorescent  $\epsilon$ -Cytidine System. *J. Am. Chem. Soc.* **1976**, *98*, 7401-7408.

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INDYLI: Indenyl lithium tetramethylethylenediamine. Rhine, W. E.; Stucky, G. D. Unsaturated Compounds of Main Group Elements - Indenyllithium Tetramethylethylenediamine. *J. Am. Chem. Soc.* **1975**, *97*, 737-743.

JOZCIK: *bis*(Pyridinium) *bis*(citrate)-chromium(III) tetrahydrate. Quiros, M.; Goodgame, D. M. L.; Williams, D. J.; Crystal Structure and EPR Spectrum of Bispyridinium *bis*(citrate)-chromium(III) Tetrahydrate. *Polyhedron* **1992**, *11*, 1343-1348.

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MEDOUR: 6-Methyl-2'-deoxyuridine. Birnbaum, G. I.; Hruska, F. E.; Niemczura, W. P. A Pyrimidine Nucleoside Constrained in the Syn Form - Structure and Conformation of 6-Methyl-2'-Deoxyuridine. *J. Am. Chem. Soc.* **1980**, *102*, 5586-5590.

NAPHTA10: Naphthalene. Brock, C. P.; Dunitz, J. D. Temperature Dependence of Thermal Motion in Crystalline Naphthalene. *Acta Crystallogr.* **1982**, *B38*, 2218-2228.

NEDDIJ: 8-Methyl-7-deaza-2'-deoxyguanosine monohydrate. Seela, F.; Rosemeyer, H.; Zulauf, M.; Chen, Y.; Kastner, G.; Reuter, H. 7-Nitro-7-deaza-2'-Deoxyadenosine and 8-Methyl-7-deaza-2'-Deoxyguanosine: Pyrrolo[2,3-d]pyrimidine Nucleosides with Different Sugar Conformations. *Liebigs Ann. Rec.* **1997**, 2525-2530.

OBNZQU: *o*-Benzoquinone. Macdonal, A. L.; Trotter, J. Crystal and Molecular Structure of *o*-Benzoquinone. *J. Chem. Soc. Perkin Trans. 2* **1973**, 476-480.

PHALIM01: Phthalimide. Ng, S. W. Structure of 1*H*-Isoindole-1,3-(2*H*)-dione (Phthalimide). *Acta Crystallogr.* **1992**, C48, 1694-1695.

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PYRDNA01: Pyridine. Mootz, D.; Wussow, H.-G. Crystal Structures of Pyridine and Pyridine Trihydrate. *J. Chem. Phys.* **1981**, 75, 1517-1522.

RIBFIM: *N*-( $\beta$ -*D*-Ribofuranosyl)imidazole. M. N. G. James, M. Matsushima, Molecular and Crystal Structure of *N*-( $\beta$ -*D*-Ribofuranosyl)imidazole. *Acta Crystallogr.* **1973**, B29, 838-846.

SECKEQ: 6-Propylcytidine. Birnbaum, K. B.; Shugar, D.; Felczak, K. 1-( $\beta$ -*D*-Ribofuranosyl)-6-Propylcytosine. *Acta Crystallogr.* **1988**, C54, 1959-1961.

SEDQEX: *N*<sup>4</sup>-5-Dimethyl-2'-deoxycytidine. Audette, G. F.; Kumar, S. V. P.; Gupta, S. V.; Quail, J. W. *N*<sup>4</sup>-5-Dimethyl-2'-deoxycytidine. *Acta Crystallogr.* **1998**, C54, 1987-1990.

SEHXAE: *tris*(Pyrimidinium) phosphododecamolybdate trihydrate. Ugalde, M.; Gutierrez-Zorrilla, J. M.; Vitoria, P.; Luque, A.; Wery, A. S. J.; Roman, P. Synthesis, Cristal Structure, and Thermal Behavior of Organically Templated Three-Dimensional Tunnel Structures Based On  $\alpha$ -Keggin Phosphododecamolybdate and Diazines. *Chem. Mat.* **1997**, *9*, 2869-2875.

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SURLOG: *tris*(Dimethylamino)sulfonium *bis*( $\eta^5$ -cyclopentadienyl)-lithium. Wessel, J.; Lork, E.; Mews, R. Alkali Metallocene Anions - Syntheses and Structures. *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 2376-2378.

TALJAR: 5-Methylcytidine. Padmaja, N.; Ramakumar, S.; Viswamitra, M. A. Structure of 5-methylcytidine. *Acta Crystallogr.* **1991**, *C47*, 1445-1448.

TAWMUZ: 1-Deoxy-1-phenyl- $\beta$ -D-ribofuranose. Matulić-Adamić, J.; Beigelman, L.; Portmann, S.; Egli, M.; Usman, N. Synthesis and Structure of 1-Deoxy-1-phenyl- $\beta$ -D-ribofuranose and Its Incorporation into Oligonucleotides *J. Org. Chem.* **1996**, *61*, 3909-3911.

TEJNIF: 4-Amino-1-(2-deoxy- $\beta$ -D-ribofuranosyl)-6,7-dihydro-1*H*,5*H*-cyclopentapyrimidine-2-one. Neidle, S.; Capaldi, D. C.; Reese, C. B.; Roselt, P. D. 4-Amino-1-(2-deoxy- $\beta$ -D-ribofuranosyl)-6,7-dihydro-1*H*,5*H*-cyclopentapyrimidine-2-one. *Acta Crystallogr.* **1996**, *C52*, 2332-2334.

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TUPQOK:  $\alpha$ -1-Naphthyl-1,2-deoxyribofuranose. Ren, R. X.-F.; Chaudhuri, N. C.; Paris, P. L.; Rumney, S. IV; Kool, E. T. Naphthalene, phenanthrene, and pyrene as DNA base analogues: Synthesis, structure, and fluorescence in DNA. *J. Am. Chem. Soc.* **1996**, *118*, 7671-7678.

VEXDOR: 5-Methoxymethyl-2'-deoxycytidine. Jia, Z.; Tourigny, G.; Delbaere, L. T. J.; Stuart, A. L.; Gupta, S. V. Structure and Conformation of 5-Methoxymethyl-2'-Deoxycytidine. *Can. J. Chem.* **1990**, *68*, 836-841.

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ZAYTIC: 3-Methyluridine. Partridge, B. L.; Pritchard, C. E. Two Methylated Ribonucleosides: 3-Methyluridine and 1-Methylinosine. *Acta Crystallogr.* **1995**, *C51*, 1929-1932.

ZIRFOV02: Pentahydrido-*tris*(triphenylphosphine)-rhenium benzene indole solvate: Patel, B. P.; Wessel, J.; Yao, W.; Lee, J. C., Jr.; Peris, E.; Koetzle, T. F.; Yap, G. P. A.; Fortin, J. B.; Ricci, J. S.; Sini, G.; Albinati, A.; Eisenstein, O.; Rheingold, A. L.; Crabtree, R. H. Intermolecular N-H...Re Interactions Involving Rhenium Polyhydrides. *New J. Chem.* **1997**, *21*, 413-421.

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**Table I.** QSPR Data<sup>a</sup> for Nucleobases in Set I

No	bn	bl	$p_p$	$p_{wkr}$	$p_{wco}$	$p_{wdg}$	$p_{cr}$	$p_m$	$p_s$	$n$	$Q$	$d_{exp}$ /Å <sup>b</sup>	$d_{HF}$ /Å	$d_{PM3}$ /Å	$d_{PLS}$ /Å
1	1	a	0.3333	0.2324	0.2308	0.2204	0.2307	0.2820	0.2307	3	13	1.367(1) 1.365(1) <b>1.367(1)</b>	1.350	1.401	1.359
	2	b	0.6667	0.7676	0.7692	0.7796	0.7432	0.7049	0.7432	2	12	1.339(1) 1.339(1) <b>1.356(1)</b>	1.343	1.359	1.367
	3	c	0.3333	0.2324	0.2308	0.2204	0.2823	0.3078	0.2823	3	12	1.425(1) 1.424(1) <b>1.428(1)</b>	1.436	1.444	1.423
	4	d	0.3333	0.3941	0.3949	0.3996	0.4871	0.4102	0.4871	2	13	1.335(2) 1.333(2) <b>1.334(1)</b>	1.342	1.404	1.346
	5	e	0.3333	0.3735	0.3743	0.3800	0.4354	0.3843	0.3333	3	13	1.335(1) 1.337(1) <b>1.343(1)</b>	1.303	1.332	1.351
	6	f	0.3333	0.2521	0.2513	0.2511	0.2307	0.2820	0.2307	3	13	1.353(1) 1.355(1) <b>1.355(1)</b>	1.350	1.417	1.359
	7	g	0.5000	0.6163	0.6173	0.6134	0.6382	0.5691	0.6382	2	14	1.240(1) 1.238(1) <b>1.250(1)</b>	1.209	1.219	1.252
	8	h	0.1667	0.1316	0.1314	0.1355	0.0641	0.1154	0.0641	4	13	1.397(2) 1.397(2) <b>1.390(1)</b>	1.402	1.459	1.379
2	9	a	0.2857	0.2114	0.2111	0.2023	0.1831	0.2344	0.1831	3	13	1.365(2) 1.367(2) <b>1.369(3)</b>	1.343	1.388	1.367
	10	b	0.7143	0.7886	0.7889	0.7977	0.7908	0.7526	0.7908	2	12	1.346(2) 1.340(2) <b>1.339(3)</b>	1.358	1.370	1.359
	11	c	0.2857	0.2114	0.2111	0.2023	0.2347	0.2602	0.2347	3	12	1.413(1) 1.413(1) <b>1.412(3)</b>	1.409	1.427	1.431
	12	d	0.4286	0.4899	0.4875	0.4977	0.5824	0.5055	0.5824	2	13	1.315(2) 1.314(2) <b>1.307(3)</b>	1.316	1.361	1.331
	13	e	0.2857	0.2987	0.3014	0.3000	0.3883	0.3370	0.2857	3	13	1.353(2) 1.352(2) <b>1.358(3)</b>	1.344	1.392	1.359
	14	f	0.2857	0.1927	0.1923	0.1927	0.1831	0.2344	0.1831	3	13	1.384(2) 1.376(2) <b>1.368(3)</b>	1.391	1.447	1.367
	15	g	0.4286	0.5928	0.5931	0.5899	0.5668	0.4977	0.5668	2	14	1.212(1) 1.217(1) <b>1.214(3)</b>	1.186	1.213	1.264
	16	h	0.2857	0.2145	0.2146	0.2147	0.1831	0.2344	0.1831	4	13	1.381(2) 1.380(2) <b>1.381(3)</b>	1.374	1.440	1.361
3	17	a	0.1429	0.0858	0.0858	0.0821	0.0403	0.0916	0.0403	3	13	1.378(1) 1.380(1) <b>1.370(3)</b>	1.381	1.414	1.390
	18	b	0.5714	0.6670	0.6716	0.6916	0.6224	0.5969	0.6224	3	12	1.339(1) 1.339(1) <b>1.341(3)</b>	1.332	1.352	1.377
	19	c	0.2857	0.2472	0.2426	0.2264	0.1837	0.2347	0.1837	2	12	1.496(1) 1.498(1)	1.502	1.483	1.441

																				<b>1.495(3)</b>
	20	d	0.1429	0.0858	0.0858	0.0821	0.1174	0.1301	0.1174	4	12	1.445(1)	1.465	1.472	1.445					<b>1.445(1)</b>
																				<b>1.447(3)</b>
	21	e	0.7143	0.7894	0.7882	0.7889	0.8525	0.7834	0.8525	2	14	1.228(1)	1.196	1.220	1.218					<b>1.228(1)</b>
																				<b>1.226(3)</b>
	22	f	0.1429	0.1248	0.1261	0.1290	0.0403	0.0916	0.1429	3	13	1.382(1)	1.385	1.430	1.382					<b>1.382(1)</b>
																				<b>1.367(3)</b>
	23	g	0.1429	0.1210	0.1223	0.1242	0.0403	0.0916	0.0403	3	13	1.373(1)	1.368	1.419	1.390					<b>1.373(1)</b>
																				<b>1.367(3)</b>
	24	h	0.7143	0.7592	0.7567	0.7528	0.8525	0.7834	0.8525	2	14	1.220(1)	1.199	1.225	1.218					<b>1.220(1)</b>
																				<b>1.219(1)</b>
																				<b>1.212(3)</b>
	25	i	0.1429	0.1429	0.1210	0.1230	0.0403	0.0916	0.0403	4	13	1.376(1)	1.371	1.437	1.383					<b>1.376(1)</b>
																				<b>1.374(1)</b>
4	26	a	0.2000	0.1211	0.1205	0.1134	0.0947	0.1474	0.0947	3	13	1.375(1)	1.382	1.418	1.381					<b>1.370(4)</b>
																				<b>1.374(1)</b>
																				<b>1.370(4)</b>
	27	b	0.8000	0.8789	0.8795	0.8866	0.8765	0.8382	0.8765	2	12	1.337(1)	1.329	1.346	1.346					<b>1.337(1)</b>
																				<b>1.332(4)</b>
	28	c	0.2000	0.1211	0.1205	0.1134	0.1490	0.1745	0.1490	3	12	1.431(1)	1.458	1.465	1.445					<b>1.431(1)</b>
																				<b>1.430(1)</b>
																				<b>1.423(4)</b>
	29	d	0.6000	0.7064	0.7063	0.7123	0.7382	0.6691	0.7382	2	14	1.232(1)	1.194	1.220	1.237					<b>1.232(1)</b>
																				<b>1.231(1)</b>
																				<b>1.232(4)</b>
	30	e	0.2000	0.1725	0.1732	0.1743	0.0974	0.1487	0.2000	3	13	1.380(1)	1.389	1.430	1.373					<b>1.380(1)</b>
																				<b>1.381(1)</b>
																				<b>1.387(4)</b>
	31	f	0.2000	0.1599	0.1606	0.1600	0.0974	0.1487	0.0974	2	13	1.373(1)	1.368	1.420	1.387					<b>1.373(1)</b>
																				<b>1.374(1)</b>
																				<b>1.371(4)</b>
	32	g	0.6000	0.6844	0.6830	0.6838	0.7382	0.6691	0.7382	2	14	1.219(1)	1.196	1.224	1.237					<b>1.219(1)</b>
																				<b>1.219(1)</b>
																				<b>1.227(4)</b>
	33	h	0.2000	0.1557	0.1564	0.1561	0.0974	0.1487	0.0974	4	13	1.381(1)	1.383	1.443	1.374					<b>1.381(1)</b>
																				<b>1.380(1)</b>
																				<b>1.376(4)</b>
5	34	a	0.3000	0.2874	0.2864	0.2851	0.2231	0.2616	0.3000	4	13	1.374(1)	1.367	1.412	1.350					<b>1.374(1)</b>
																				<b>1.370(2)</b>
																				<b>1.371(2)</b>
	35	b	0.3000	0.2520	0.2534	0.2507	0.1974	0.2487	0.1974	3	13	1.373(1)	1.376	1.424	1.365					<b>1.373(1)</b>
																				<b>1.374(1)</b>
																				<b>1.373(2)</b>
																				<b>1.375(2)</b>
	36	c	0.7000	0.7480	0.7466	0.7493	0.8282	0.7641	0.8282	2	13	1.311(1)	1.279	1.334	1.289					<b>1.311(1)</b>
																				<b>1.311(1)</b>
																				<b>1.313(2)</b>
																				<b>1.314(2)</b>
	37	d	0.1000	0.0762	0.0762	0.0751	-0.2600	0.0487	0.0000	3	13	1.388(1)	1.383	1.412	1.396					<b>1.388(1)</b>
																				<b>1.388(1)</b>
																				<b>1.387(2)</b>
																				<b>1.390(2)</b>
	38	e	0.4000	0.4475	0.4483	0.4525	0.4225	0.4113	0.4225	4	12	1.383(1)	1.376	1.415	1.401					<b>1.383(1)</b>



											1.382(1)				
											1.393(2)				
											1.394(2)				
39	f	0.4000	0.3809	0.3809	0.3789	0.3745	0.3872	0.3745	4	12	1.406(1)	1.400	1.415	1.404	
											1.406(1)				
											1.415(2)				
											1.416(2)				
40	g	0.2000	0.2415	0.2412	0.2445	0.3538	0.2769	0.3538	2	13	1.335(1)	1.344	1.397	1.367	
											1.336(1)				
											1.335(2)				
											1.335(2)				
41	h	0.4000	0.3777	0.3779	0.3765	0.2974	0.3487	0.4000	3	13	1.351(1)	1.328	1.366	1.341	
											1.352(1)				
											1.355(2)				
											1.357(2)				
42	i	0.4000	0.4020	0.4022	0.4017	0.4000	0.4000	0.4000	2	13	1.339(1)	1.328	1.370	1.347	
											1.340(1)				
											1.339(2)				
											1.340(2)				
43	j	0.6000	0.5980	0.5978	0.5983	0.6000	0.6000	0.6000	2	13	1.331(1)	1.313	1.348	1.315	
											1.330(1)				
											1.334(2)				
											1.335(2)				
44	k	0.2000	0.1889	0.1892	0.1874	0.2000	0.2000	0.0974	3	13	1.344(1)	1.328	1.374	1.381	
											1.345(1)				
											1.345(2)				
											1.348(2)				
6	45	a	0.3000	0.2913	0.2902	0.2878	0.3000	0.3000	0.3000	4	13	1.365(2)	1.343	1.394	1.350
											1.360(2)				
											1.362(4)				
46	b	0.3000	0.2485	0.2500	0.2472	0.1974	0.2487	0.1974	3	13	1.373(2)	1.381	1.421	1.365	
											1.372(2)				
											1.381(4)				
47	c	0.7000	0.7515	0.7500	0.7528	0.8282	0.7641	0.8282	2	13	1.312(2)	1.284	1.340	1.289	
											1.310(2)				
											1.307(5)				
48	d	0.1000	0.0791	0.0790	0.0777	-0.2600	0.0487	0.0000	3	13	1.379(1)	1.369	1.403	1.396	
											1.379(1)				
											1.375(4)				
49	e	0.4000	0.4652	0.4650	0.4719	0.4255	0.4128	0.4255	4	12	1.378(2)	1.380	1.417	1.400	
											1.376(2)				
											1.385(4)				
50	f	0.4000	0.3566	0.3580	0.3535	0.3745	0.3872	0.3745	4	12	1.403(2)	1.390	1.418	1.404	
											1.402(2)				
											1.398(4)				
51	g	0.2000	0.2526	0.2517	0.2566	0.3538	0.2769	0.3538	2	13	1.320(2)	1.319	1.363	1.367	
											1.315(2)				
											1.326(4)				
52	h	0.4000	0.3908	0.3903	0.3899	0.4000	0.4000	0.4000	3	13	1.359(2)	1.358	1.401	1.341	
											1.362(2)				
											1.351(4)				
53	i	0.4000	0.3627	0.3651	0.3609	0.2718	0.3359	0.4000	2	13	1.357(2)	1.372	1.421	1.347	
											1.358(2)				
											1.360(5)				
54	j	0.6000	0.6373	0.6349	0.6391	0.7282	0.6641	0.6000	2	13	1.305(2)	1.274	1.316	1.315	
											1.302(2)				
											1.308(5)				
55	k	0.2000	0.1644	0.1658	0.1626	0.0974	0.1487	0.0974	3	13	1.356(1)	1.350	1.393	1.381	
											1.355(1)				
											1.353(4)				

7	56	a	0.1000	0.0782	0.0777	0.0780	0.0231	0.0616	0.1000	4	13	1.375(2)	1.355	1.402	1.382
												<i>1.375(2)</i>			
												<b>1.379(6)</b>			
	57	b	0.2000	0.1825	0.1840	0.1813	0.0974	0.1487	0.0974	3	13	1.374(1)	1.378	1.420	1.381
												<i>1.374(1)</i>			
												<b>1.382(6)</b>			
	58	c	0.8000	0.8175	0.8160	0.8187	0.9282	0.8641	0.9282	2	13	1.305(1)	1.280	1.339	1.273
												<i>1.306(1)</i>			
												<b>1.300(6)</b>			
	59	d	0.1000	0.0817	0.0818	0.0798	-0.2600	0.0487	0.0000	3	13	1.388(1)	1.374	1.400	1.396
												<i>1.387(1)</i>			
												<b>1.389(6)</b>			
	60	e	0.5000	0.5551	0.5573	0.5639	0.5255	0.5128	0.5255	4	12	1.379(2)	1.367	1.403	1.384
												<i>1.379(2)</i>			
												<b>1.374(6)</b>			
	61	f	0.2000	0.1571	0.1562	0.1563	0.1745	0.1873	0.1745	4	12	1.419(2)	1.436	1.448	1.436
												<i>1.417(2)</i>			
												<b>1.420(6)</b>			
	62	g	0.7000	0.7584	0.7597	0.7571	0.8382	0.7691	0.8382	2	14	1.237(2)	1.193	1.216	1.221
												<i>1.238(2)</i>			
												<b>1.234(6)</b>			
	63	h	0.1000	0.0844	0.0841	0.0867	-0.2600	0.0487	0.1000	3	13	1.391(1)	1.417	1.455	1.388
												<i>1.392(1)</i>			
												<b>1.390(6)</b>			
	64	i	0.2000	0.2070	0.2073	0.2059	0.2026	0.2026	0.2000	3	13	1.373(2)	1.359	1.412	1.373
												<i>1.372(2)</i>			
												<b>1.370(6)</b>			
	65	j	0.3000	0.3119	0.3111	0.3095	0.4538	0.3769	0.4538	2	13	1.341(2)	1.360	1.422	1.351
												<i>1.340(2)</i>			
												<b>1.339(6)</b>			
	66	k	0.5000	0.4811	0.4816	0.4846	0.3974	0.4487	0.5000	3	13	1.323(2)	1.289	1.340	1.325
												<i>1.323(2)</i>			
												<b>1.323(6)</b>			
	67	l	0.3000	0.2850	0.2833	0.2783	0.1974	0.2487	0.1974	3	13	1.350(2)	1.359	1.397	1.365
												<i>1.351(2)</i>			
												<b>1.354(6)</b>			

<sup>a</sup>The nucleobase numeration from Figure 2 and Table 1. The bond length numeration (bn, bl) is according to Figure 2. See the text for the definition of the bond orders  $p_p$ ,  $p_{wkr}$ ,  $p_{wco}$ ,  $p_{wdg}$ ,  $p_{cr}$ ,  $p_m$ ,  $p_s$ , descriptors  $n$  and  $Q$ . Bond lengths: experimental ( $d_{exp}$ ), with esds in parentheses, from HF ( $d_{HF}$ ), PM3 ( $d_{PM3}$ ) and PLS - ( $d_{PLS}$ , model 34) calculations. <sup>b</sup>Experimental bond lengths: from work of Berman *et al.*<sup>11</sup> (plain); updated by Berman *et al.*<sup>43</sup> (italics); from nucleoside crystal structures uncorrected (bold) and corrected (underlined) to libration motion in crystal.

Table II. QSPR Data<sup>a</sup> for Nucleobases in Set II

No	bn	bl	$p_p$	$p_{wkr}$	$p_{wco}$	$p_{wdg}$	$p_{cr}$	$p_m$	$p_s$	$n$	$Q$	$d_{exp}$ /Å <sup>b</sup>	$d_{HF}$ /Å	$d_{PM3}$ /Å	$d_{PLS}$ /Å
8	68	a	0.1250	0.12	0.1194	0.1169	0.0224	0.0224	0.1250	3	13	1.373(1) <i>1.374(1)</i>	1.357	1.396	1.384
	69	b	0.7500	0.7297	0.7294	0.7302	0.6218	0.6859	0.6218	2	13	1.327(2) <i>1.327(2)</i>	1.298	1.350	1.302
	70	c	0.2500	0.2703	0.2706	0.2698	0.3526	0.3013	0.3526	3	13	1.358(1) <i>1.360(1)</i>	1.351	1.402	1.357
	71	d	0.1250	0.1325	0.1308	0.1296	0.1250	0.1250	0.0481	4	13	1.383(1) <i>1.383(1)</i>	1.380	1.411	1.384
	72	e	0.5000	0.5583	0.5601	0.5692	0.5255	0.5128	0.5255	4	12	1.382(2) <i>1.383(2)</i>	1.368	1.437	1.384
	73	f	0.1250	0.0773	0.0774	0.0761	0.0995	0.1123	0.0995	4	12	1.429(1) <i>1.430(1)</i>	1.432	1.448	1.448
	74	g	0.7500	0.8275	0.8277	0.8257	0.8882	0.8191	0.8882	2	14	1.229(2) <i>1.230(2)</i>	1.203	1.226	1.213
	75	h	0.1250	0.0953	0.0949	0.0982	0.0224	0.0737	0.1250	3	13	1.400(1) <i>1.401(1)</i>	1.390	1.431	1.384
	76	i	0.3750	0.3231	0.3255	0.3190	0.2468	0.3109	0.3750	2	13	1.359(2) <i>1.360(2)</i>	1.366	1.413	1.351
	77	j	0.6250	0.6769	0.6745	0.6810	0.7532	0.6891	0.6250	2	13	1.307(1) <i>1.308(1)</i>	1.269	1.314	1.311
78	k	0.2500	0.1892	0.1896	0.1843	0.1474	0.1987	0.1474	3	13	1.366(2) <i>1.366(2)</i>	1.371	1.403	1.373	
9	79	a	0.1667	0.0953	0.0950	0.0901	0.0641	0.1154	0.0641	3	13	1.378(1)	1.383	1.410	1.386
	80	b	0.6667	0.7591	0.7626	0.7779	0.7177	0.6922	0.7177	3	12	1.351(1)	1.330	1.353	1.362
	81	c	0.1667	0.1455	0.1424	0.1320	0.1157	0.1412	0.1157	3	12	1.495(1)	1.512	1.503	1.450
	82	d	0.1667	0.0953	0.0950	0.0901	0.1412	0.1539	0.1412	4	12	1.455(1)	1.463	1.469	1.441
	83	e	0.6667	0.7730	0.7724	0.7757	0.8049	0.7358	0.8049	2	14	1.227(1)	1.196	1.221	1.226
	84	f	0.1667	0.1316	0.1326	0.1342	0.0641	0.1154	0.1667	3	13	1.391(1)	1.384	1.431	1.378
	85	g	0.1667	0.1467	0.1479	0.1490	0.0641	0.1154	0.0641	3	13	1.368(1)	1.369	1.418	1.386
	86	h	0.6667	0.7128	0.7105	0.7081	0.8049	0.7358	0.8049	2	14	1.230(1)	1.197	1.225	1.226
	87	i	0.1667	0.1405	0.1416	0.1429	0.0641	0.1154	0.0641	4	13	1.379(1)	1.377	1.440	1.379
10	88	a	0.2222	0.1465	0.1472	0.1394	0.1196	0.1709	0.1196	3	13	1.368(5)	1.363	1.403	1.377
	89	b	0.5556	0.6645	0.6680	0.6849	0.6066	0.5811	0.6066	3	12	1.347(6)	1.340	1.363	1.380
	90	c	0.2222	0.1890	0.1847	0.1756	0.1712	0.1967	0.1712	2	12	1.490(5)	1.504	1.483	1.447
	91	d	0.2222	0.1465	0.1472	0.1394	0.1967	0.2095	0.1967	4	12	1.431(5)	1.443	1.452	1.433
	92	e	0.2222	0.1920	0.1957	0.1954	0.1152	0.1687	0.3292	3	14	1.325(5)	1.316	1.358	1.293
	93	f	0.5556	0.6615	0.6570	0.6651	0.6582	0.6069	0.5556	3	13	1.306(5)	1.281	1.323	1.316
	94	g	0.2222	0.1381	0.1396	0.1373	0.1196	0.1709	0.2222	3	13	1.356(5)	1.369	1.423	1.369
	95	h	0.6667	0.7693	0.7676	0.7669	0.8049	0.7358	0.8049	2	14	1.233(5)	1.199	1.217	1.226
	96	i	0.1111	0.0926	0.0928	0.0958	0.0342	0.0727	0.0342	4	13	1.386(4)	1.398	1.456	1.386
11	97	a	0.1667	0.0940	0.0944	0.0902	0.0641	0.1154	0.0641	3	13	1.349(3)	1.356	1.397	1.386
	98	b	0.8333	0.9060	0.9056	0.9098	0.9098	0.8716	0.9098	2	12	1.347(4)	1.343	1.362	1.340
	99	c	0.1667	0.0940	0.0944	0.0902	0.1157	0.1412	0.1157	3	12	1.402(4)	1.431	1.441	1.450
	100	d	0.3333	0.2493	0.2532	0.2503	0.2263	0.2798	0.4403	3	14	1.338(3)	1.313	1.358	1.275
	101	e	0.5000	0.6568	0.6525	0.6595	0.6026	0.5513	0.5000	3	13	1.299(3)	1.289	1.328	1.325
	102	f	0.3333	0.1926	0.1941	0.1895	0.2307	0.2820	0.2307	2	13	1.362(3)	1.359	1.418	1.366
	103	g	0.5000	0.6861	0.6853	0.6864	0.6387	0.5694	0.6387	2	14	1.226(3)	1.207	1.222	1.252
	104	h	0.1667	0.1213	0.1206	0.1241	0.0898	0.1283	0.0898	4	13	1.402(3)	1.395	1.456	1.377
12	105	a	0.2500	0.1752	0.1750	0.1700	0.1731	0.2116	0.1731	4	13	1.388(2) <i>1.390(2)</i>	1.376	1.416	1.364
	106	b	0.2500	0.1985	0.1944	0.1865	0.1990	0.2245	0.1990	3	12	1.513(4) <i>1.517(4)</i>	1.515	1.504	1.437
	107	c	0.5000	0.6263	0.6306	0.6435	0.5510	0.5255	0.5510	3	12	1.340(3) <i>1.341(3)</i>	1.346	1.367	1.389
	108	d	0.2500	0.1752	0.1750	0.1700	0.1990	0.2245	0.1990	3	12	1.425(3) <i>1.429(3)</i>	1.434	1.438	1.437

	109	e	0.2500	0.3327	0.3346	0.3416	0.4038	0.3269	0.4038	2	13	1.323(3)	1.342	1.405	1.359
												1.324(3)			
	110	f	0.5000	0.4921	0.4905	0.4884	0.5000	0.5000	0.5000	3	13	1.331(2)	1.296	1.329	1.325
												1.333(2)			
	111	g	0.2500	0.2044	0.2044	0.2073	0.1474	0.1987	0.1474	3	13	1.345(3)	1.353	1.416	1.373
												1.347(3)			
	112	h	0.6250	0.6949	0.6947	0.6872	0.7632	0.6941	0.7632	2	14	1.237(2)	1.203	1.220	1.233
												1.239(2)			
	113	i	0.1250	0.17	0.1010	0.1055	0.0481	0.0866	0.0481	4	13	1.408(3)	1.414	1.462	1.384
												1.412(3)			
<b>13</b>	114	a	0.1875	0.1992	0.1981	0.1984	0.2644	0.2260	0.1875	4	13	1.369(3)	1.351	1.402	1.368
	115	b	0.3750	0.3557	0.3576	0.3559	0.2724	0.3237	0.2724	3	13	1.361(3)	1.374	1.411	1.353
	116	c	0.6250	0.6443	0.6424	0.6441	0.7532	0.6891	0.7532	2	13	1.313(3)	1.288	1.348	1.301
	117	d	0.1875	0.1669	0.1672	0.1651	0.0849	0.1362	0.0849	3	13	1.375(3)	1.364	1.392	1.383
	118	e	0.3750	0.4156	0.4154	0.4210	0.4500	0.3878	0.4500	4	12	1.389(3)	1.381	1.420	1.404
	119	f	0.2500	0.2151	0.2166	0.2136	0.2245	0.2373	0.2245	4	12	1.399(3)	1.389	1.411	1.428
	120	g	0.2500	0.2669	0.2665	0.2689	0.3269	0.2884	0.2500	4	13	1.367(3)	1.356	1.407	1.358
	121	h	0.3750	0.4216	0.4207	0.4234	0.4519	0.4134	0.4519	3	13	1.335(3)	1.329	1.381	1.339
	122	i	0.1250	0.0966	0.0951	0.0934	-0.3200	0.0609	0.1250	2	13	1.389(3)	1.387	1.409	1.391
	123	j	0.8750	0.9034	0.9049	0.9066	0.9515	0.9133	0.8750	3	12	1.327(3)	1.331	1.379	1.333
	124	k	0.1250	0.0966	0.0951	0.0934	0.0224	0.0737	0.1250	3	13	1.397(3)	1.407	1.413	1.384
	125	l	0.3750	0.3389	0.3425	0.3378	0.2724	0.3237	0.3750	3	13	1.374(3)	1.373	1.425	1.345
	126	m	0.6250	0.6611	0.6575	0.6622	0.6250	0.6250	0.5485	2	13	1.294(3)	1.275	1.315	1.317
	127	n	0.2500	0.2181	0.2203	0.2163	0.1218	0.1859	0.1218	3	13	1.352(3)	1.347	1.392	1.375
<b>14</b>	128	a	0.2500	0.1490	0.1488	0.1430	0.1474	0.1987	0.1474	3	13	1.373(2)	1.359	1.400	1.373
	129	b	0.7500	0.8510	0.8512	0.8570	0.8265	0.7883	0.8265	2	12	1.350(2)	1.342	1.358	1.354
	130	c	0.2500	0.1490	0.1488	0.1430	0.1990	0.2245	0.1990	3	12	1.426(2)	1.438	1.439	1.437
	131	d	0.2500	0.2034	0.2037	0.2016	0.0962	0.1731	0.4038	2	13	1.358(2)	1.364	1.418	1.359
	132	e	0.5000	0.6476	0.6475	0.6554	0.5510	0.5255	0.5000	3	12	1.371(2)	1.364	1.368	1.393
	133	f	0.5000	0.3524	0.3525	0.3446	0.4490	0.4745	0.4490	3	12	1.418(2)	1.427	1.450	1.397
	134	g	0.2500	0.4364	0.4350	0.4342	0.3882	0.3191	0.3882	2	14	1.243(2)	1.220	1.229	1.292
	135	h	0.2500	0.2112	0.2125	0.2212	0.1731	0.2116	0.1731	4	13	1.405(2)	1.392	1.445	1.364
<b>15</b>	136	a	0.7143	0.8462	0.8489	0.8540	0.7653	0.7398	0.6633	3	12	1.342(5)	1.327	1.351	1.363
	137	b	0.2857	0.1538	0.1511	0.1460	0.1575	0.2216	0.4139	2	13	1.372(5)	1.403	1.418	1.355
	138	c	0.2857	0.3103	0.3114	0.3126	0.3883	0.3370	0.1831	3	13	1.332(5)	1.325	1.387	1.367
	139	d	0.4286	0.4233	0.4209	0.4248	0.4286	0.4286	0.5051	2	13	1.317(5)	1.321	1.390	1.337
	140	e	0.2857	0.2664	0.2677	0.2626	0.1831	0.2344	0.2857	3	13	1.348(5)	1.327	1.384	1.359
	141	f	0.2857	0.1968	0.1950	0.2300	0.1831	0.2344	0.1831	3	13	1.408(5)	1.428	1.470	1.367
	142	g	0.4286	0.6494	0.6539	0.6537	0.5668	0.4977	0.5668	2	14	1.213(5)	1.180	1.206	1.264
	143	h	0.2857	0.1538	0.1511	0.1460	0.2602	0.2730	0.2602	4	12	1.452(5)	1.465	1.472	1.422
<b>16</b>	144	a	0.2000	0.1269	0.1264	0.1182	0.0974	0.1487	0.0974	3	13	1.370(3)	1.374	1.415	1.381
												1.374(3)			
	145	b	0.8000	0.8731	0.8736	0.8818	0.8765	0.8382	0.8765	2	12	1.339(4)	1.328	1.345	1.346
												1.341(4)			
	146	c	0.2000	0.1269	0.1264	0.1182	0.1490	0.1745	0.1490	3	12	1.433(4)	1.457	1.468	1.445
												1.437(4)			
	147	d	0.6000	0.6955	0.6953	0.7010	0.7382	0.6691	0.7382	2	14	1.241(3)	1.195	1.220	1.237
												1.242(3)			
	148	e	0.2000	0.1775	0.1784	0.1808	0.1231	0.1616	0.2000	4	13	1.390(3)	1.401	1.441	1.366
												1.395(3)			
	149	f	0.2000	0.1396	0.1405	0.1394	0.1231	0.1616	0.1231	4	13	1.390(3)	1.369	1.430	1.372
												1.392(3)			
	150	g	0.6000	0.7191	0.7172	0.7198	0.7382	0.6691	0.7382	2	14	1.210(3)	1.204	1.223	1.237
												1.215(3)			
	151	h	0.2000	0.1413	0.1422	0.1408	0.1231	0.1616	0.1231	4	13	1.386(3)	1.375	1.447	1.372
												1.390(3)			
<b>17</b>	152	a	0.2500	0.1747	0.1745	0.1675	0.1474	0.1987	0.1474	3	13	1.370(3)	1.358	1.400	1.373
	153	b	0.5000	0.6162	0.6212	0.6369	0.5510	0.5255	0.5510	3	12	1.344(4)	1.341	1.363	1.389
	154	c	0.2500	0.2091	0.2042	0.1956	0.1990	0.2245	0.1990	2	12	1.502(4)	1.506	1.484	1.443
	155	d	0.2500	0.1747	0.1745	0.1675	0.2245	0.2373	0.2245	4	12	1.439(4)	1.449	1.452	1.428

	156	e	0.2500	0.2826	0.2866	0.2900	0.4038	0.3269	0.4038	2	13	1.349(4)	1.346	1.405	1.359
	157	f	0.5000	0.5427	0.5389	0.5425	0.6026	0.5513	0.5000	3	13	1.320(4)	1.295	1.329	1.325
	158	g	0.2500	0.1869	0.1881	0.1883	0.1474	0.1987	0.1474	3	13	1.367(4)	1.359	1.419	1.373
	159	h	0.6250	0.6920	0.6905	0.6851	0.7632	0.6941	0.7632	2	14	1.249(3)	1.200	1.217	1.233
	160	i	0.1250	0.1211	0.1215	0.1266	0.1250	0.1250	0.0481	4	13	1.380(3)	1.407	1.460	1.384
18	161	a	0.2222	0.2062	0.2058	0.2068	0.1453	0.1838	0.2222	4	13	1.390(3)	1.376	1.416	1.363
	162	b	0.3333	0.2800	0.2821	0.2780	0.2307	0.2820	0.2307	3	13	1.365(3)	1.370	1.421	1.359
	163	c	0.6667	0.7200	0.7179	0.7220	0.7949	0.7308	0.7949	2	13	1.310(3)	1.279	1.333	1.295
	164	d	0.1111	0.0755	0.0776	0.0759	0.8500	0.0598	0.8500	3	13	1.388(3)	1.383	1.414	1.395
	165	e	0.3333	0.3238	0.3245	0.3240	0.3333	0.3333	0.3588	4	12	1.397(3)	1.385	1.417	1.411
	166	f	0.3333	0.3762	0.3776	0.3811	0.3588	0.3460	0.3078	4	12	1.403(4)	1.396	1.411	1.415
	167	g	0.2222	0.2580	0.2576	0.2587	0.3760	0.2991	0.3760	2	13	1.368(3)	1.359	1.408	1.363
	168	h	0.4444	0.3658	0.3649	0.3603	0.3934	0.4189	0.4444	3	13	1.392(4)	1.398	1.400	1.334
	169	i	0.5556	0.6342	0.6351	0.6397	0.6321	0.5938	0.5556	2	12	1.386(4)	1.388	1.405	1.390
	170	j	0.4444	0.3658	0.3649	0.3603	0.3162	0.3803	0.4444	2	13	1.345(4)	1.324	1.349	1.340
	171	k	0.3333	0.3925	0.3921	0.3933	0.4359	0.3846	0.2823	3	13	1.330(3)	1.324	1.372	1.355
19	172	a	0.2857	0.3439	0.3434	0.3491	0.3883	0.3370	0.2857	3	13	1.334(5)	1.322	1.378	1.359
	173	b	0.1429	0.1111	0.1104	0.1055	0.0147	0.0788	0.0147	2	13	1.377(5)	1.396	1.416	1.398
	174	c	0.8571	0.8889	0.8896	0.8945	0.9853	0.9212	0.9853	2	12	1.326(5)	1.331	1.374	1.332
	175	d	0.1429	0.1111	0.1104	0.1055	0.0403	0.0916	0.0403	3	13	1.394(5)	1.399	1.418	1.390
	176	e	0.2857	0.3148	0.3160	0.3189	0.3112	0.2984	0.3112	4	13	1.352(5)	1.340	1.398	1.350
	177	f	0.1429	0.0841	0.0843	0.0841	0.1174	0.1301	0.1174	4	13	1.404(5)	1.406	1.459	1.377
	178	g	0.5714	0.6953	0.6943	0.6922	0.7096	0.6405	0.7096	2	14	1.207(5)	1.182	1.212	1.241
	179	h	0.2857	0.2206	0.2214	0.2238	0.2088	0.2473	0.2857	4	13	1.377(5)	1.375	1.437	1.352
	180	i	0.2857	0.2301	0.2303	0.2266	0.1831	0.2344	0.2857	3	13	1.382(5)	1.363	1.399	1.359
	181	j	0.7143	0.7699	0.7697	0.7734	0.7908	0.7526	0.7143	2	12	1.348(5)	1.350	1.367	1.365
	182	k	0.2857	0.2301	0.2303	0.2266	0.2347	0.2602	0.2347	3	12	1.393(5)	1.414	1.420	1.431
20	183	a	0.3333	0.2296	0.2272	0.2241	0.3078	0.3206	0.3333	4	12	1.421(3)	1.423	1.422	1.413
	184	b	0.6667	0.7704	0.7728	0.7759	0.7177	0.6922	0.6157	3	12	1.384(3)	1.365	1.400	1.370
	185	c	0.3333	0.2296	0.2272	0.2241	0.2051	0.2692	0.4615	2	13	1.361(3)	1.357	1.389	1.348
	186	d	0.2222	0.1563	0.1545	0.1537	0.1196	0.1709	0.1196	3	13	1.365(3)	1.362	1.397	1.377
	187	e	0.3333	0.4221	0.4240	0.4301	0.3588	0.3460	0.3588	4	12	1.394(3)	1.370	1.413	1.411
	188	f	0.3333	0.1754	0.1760	0.1763	0.3078	0.3206	0.3078	4	12	1.423(3)	1.434	1.448	1.415
	189	g	0.5556	0.7168	0.7160	0.7120	0.6938	0.6247	0.6938	2	14	1.234(3)	1.200	1.224	1.244
	190	h	0.1111	0.1078	0.1080	0.1117	0.1111	0.1111	0.1111	3	13	1.382(3)	1.391	1.430	1.387
	191	i	0.3333	0.3231	0.3278	0.3243	0.3333	0.3333	0.3333	2	13	1.367(3)	1.367	1.412	1.358
	192	j	0.6667	0.6769	0.6722	0.6757	0.6667	0.6667	0.6667	2	13	1.301(3)	1.269	1.314	1.305
	193	k	0.2222	0.1920	0.1943	0.1922	0.1196	0.1709	0.1196	3	13	1.383(3)	1.382	1.404	1.377
21	194	a	0.2000	0.1955	0.1939	0.1890	0.2000	0.2000	0.2000	4	13	1.363(4)	1.355	1.408	1.366
	195	b	0.2000	0.1945	0.1967	0.1949	0.2000	0.2000	0.0974	3	13	1.389(4)	1.385	1.425	1.381
	196	c	0.8000	0.8055	0.8033	0.8051	0.8000	0.8000	0.9026	2	13	1.313(4)	1.275	1.334	1.276
	197	d	0.1000	0.0829	0.0833	0.0810	-0.2600	0.0487	0.0000	3	13	1.393(4)	1.377	1.400	1.396
	198	e	0.5000	0.5324	0.5349	0.5466	0.5255	0.5128	0.5255	4	12	1.371(4)	1.356	1.399	1.384
	199	f	0.2000	0.1434	0.1432	0.1405	0.1745	0.1873	0.1745	4	12	1.427(4)	1.450	1.457	1.436
	200	g	0.7000	0.7782	0.7782	0.7793	0.8382	0.7691	0.8382	2	14	1.216(4)	1.191	1.215	1.221
	201	h	0.1000	0.0783	0.0786	0.0802	-0.2600	0.0487	0.1000	3	13	1.399(4)	1.405	1.444	1.388
	202	i	0.1000	0.0871	0.0875	0.0893	-0.2600	0.0487	0.1000	3	13	1.383(4)	1.373	1.421	1.388
	203	j	0.8000	0.8242	0.8235	0.8200	0.9382	0.8691	0.9382	2	14	1.227(4)	1.197	1.227	1.205
	204	k	0.1000	0.0886	0.0890	0.0907	-0.2600	0.0487	0.1000	3	13	1.377(4)	1.372	1.433	1.388
	205	l	0.2000	0.1893	0.1879	0.1835	0.0974	0.1487	0.0974	3	13	1.372(4)	1.363	1.407	1.381
22	206	a	0.1538	0.1565	0.1560	0.1566	0.1538	0.1538	0.1538	4	13	1.371(2)	1.357	1.401	1.373
												1.372(2)			
	207	b	0.0769	0.0655	0.0648	0.0641	0.0000	0.0384	0.0000	4	13	1.411(2)	1.405	1.429	1.392
												1.413(2)			
	208	c	0.1538	0.1404	0.1385	0.1353	0.1283	0.1411	0.1283	2	12	1.486(3)	1.496	1.475	1.456
												1.488(3)			
	209	d	0.7692	0.7941	0.7967	0.8600	0.8202	0.7947	0.8202	3	12	1.363(3)	1.347	1.388	1.346
												1.365(3)			
	210	e	0.0769	0.0655	0.0648	0.0641	0.0000	0.0384	0.0000	3	12	1.421(3)	1.432	1.423	1.466
												1.423(3)			

211	f	0.4615	0.4910	0.4911	0.4925	0.4870	0.4743	0.4870	4	12	1.394(3)	1.372	1.407	1.390	
											1.396(3)				
212	g	0.2308	0.1922	0.1930	0.1953	0.2053	0.2181	0.2053	4	12	1.417(3)	1.430	1.444	1.431	
											1.418(3)				
213	h	0.6923	0.7391	0.7380	0.7335	0.8305	0.7614	0.8305	2	14	1.246(2)	1.199	1.221	1.222	
											1.248(2)				
214	i	0.0769	0.0687	0.0689	0.0713	0.0769	0.0769	0.0769	3	13	1.389(3)	1.410	1.447	1.392	
											1.392(3)				
215	j	0.2308	0.2183	0.2201	0.2201	0.1282	0.1795	0.2308	3	13	1.377(2)	1.358	1.413	1.369	
											1.379(2)				
216	k	0.2308	0.2461	0.2472	0.2466	0.3334	0.2821	0.3334	2	13	1.341(3)	1.364	1.427	1.366	
											1.343(3)				
217	l	0.5385	0.5356	0.5328	0.5333	0.5385	0.5385	0.5385	3	13	1.321(2)	1.285	1.335	1.319	
											1.322(2)				
218	m	0.3077	0.2870	0.2881	0.2868	0.2051	0.2564	0.2051	3	13	1.357(2)	1.362	1.400	1.363	
											1.359(2)				
23	219	a	0.1667	0.1076	0.1073	0.1029	0.0641	0.1154	0.0641	3	13	1.374(3)	1.387	1.418	1.386
	220	b	0.6667	0.7394	0.7431	0.7563	0.7177	0.6922	0.7177	3	12	1.360(3)	1.331	1.352	1.362
	221	c	0.1667	0.1531	0.1495	0.1407	0.1412	0.1539	0.1412	4	12	1.504(3)	1.515	1.503	1.441
	222	d	0.1667	0.1076	0.1073	0.1029	0.1412	0.1539	0.1412	4	12	1.447(3)	1.470	1.472	1.441
	223	e	0.6667	0.7482	0.7473	0.7495	0.8049	0.7358	0.8049	2	14	1.233(3)	1.196	1.220	1.226
	224	f	0.1667	0.1442	0.1453	0.1476	0.0641	0.1154	0.1667	3	13	1.383(3)	1.384	1.431	1.378
	225	g	0.1667	0.1286	0.1297	0.1300	0.0641	0.1154	0.0641	3	13	1.378(3)	1.367	1.420	1.386
	226	h	0.6667	0.7411	0.7388	0.7384	0.8049	0.7358	0.8049	2	14	1.216(3)	1.199	1.225	1.226
	227	i	0.1667	0.1303	0.1315	0.1316	0.0898	0.1283	0.0898	4	13	1.374(3)	1.373	1.439	1.377
24	228	a	0.2500	0.1696	0.1683	0.1599	0.1474	0.1987	0.1474	3	13	1.362(3)	1.353	1.403	1.373
	229	b	0.7500	0.8304	0.8317	0.8401	0.8265	0.7883	0.8265	3	12	1.359(3)	1.349	1.358	1.347
	230	c	0.1250	0.0843	0.0834	0.0794	0.0995	0.1123	0.0995	4	12	1.494(3)	1.489	1.493	1.448
	231	d	0.6250	0.6974	0.6987	0.7036	0.7632	0.6941	0.6250	2	14	1.231(3)	1.201	1.219	1.243
	232	e	0.2500	0.2183	0.2179	0.2170	0.1735	0.2117	0.2500	4	12	1.484(4)	1.504	1.500	1.426
	233	f	0.1250	0.0853	0.0849	0.0806	0.0995	0.1123	0.0995	2	12	1.460(3)	1.461	1.468	1.461
	234	g	0.7500	0.8079	0.8077	0.8106	0.8882	0.8191	0.8882	2	14	1.223(3)	1.197	1.220	1.213
	235	h	0.1250	0.1068	0.1074	0.1088	0.0224	0.0737	0.1250	3	13	1.400(3)	1.393	1.432	1.384
	236	i	0.1250	0.1119	0.1127	0.1121	0.0224	0.0737	0.0224	3	13	1.367(3)	1.363	1.419	1.392
	237	j	0.7500	0.7890	0.7876	0.7871	0.8882	0.8191	0.8882	2	14	1.215(3)	1.195	1.223	1.213
	238	k	0.1250	0.0991	0.0997	0.1800	0.0481	0.0866	0.0481	4	13	1.406(2)	1.388	1.444	1.384
25	239	a	0.3000	0.2653	0.2646	0.2598	0.1974	0.2487	0.3000	3	13	1.352(4)	1.349	1.385	1.357
	240	b	0.6000	0.6017	0.6016	0.6046	0.6000	0.6000	0.4974	3	13	1.340(4)	1.314	1.373	1.317
	241	c	0.4000	0.3983	0.3984	0.3954	0.4000	0.4000	0.5026	3	13	1.350(4)	1.326	1.382	1.333
	242	d	0.1000	0.1035	0.1028	0.1400	0.1000	0.1000	0.0000	3	13	1.380(4)	1.379	1.402	1.396
	243	e	0.5000	0.5267	0.5288	0.5386	0.5255	0.5128	0.5255	4	12	1.369(4)	1.355	1.403	1.384
	244	f	0.2000	0.1558	0.1558	0.1544	0.1745	0.1873	0.2255	4	12	1.409(5)	1.431	1.451	1.432
	245	g	0.7000	0.7630	0.7627	0.7622	0.8382	0.7691	0.8382	2	14	1.228(4)	1.200	1.222	1.221
	246	h	0.1000	0.0812	0.0815	0.0834	0.0231	0.0616	0.1000	4	13	1.395(4)	1.399	1.442	1.382
	247	i	0.1000	0.0829	0.0831	0.0853	0.0231	0.0616	0.1000	4	13	1.398(5)	1.390	1.447	1.382
	248	j	0.8000	0.8273	0.8267	0.8229	0.9382	0.8691	0.9382	2	14	1.233(4)	1.199	1.224	1.205
	249	k	0.1000	0.0899	0.0902	0.0918	0.1000	0.1000	0.1000	4	13	1.365(4)	1.374	1.444	1.382
	250	l	0.1000	0.1045	0.1038	0.1012	0.1000	0.1000	0.0231	4	13	1.377(4)	1.370	1.416	1.388
26	251	a	0.2737	0.2522	0.2541	0.2353	0.1958	0.2348	0.1958	4	13	1.379(4)	1.365	1.403	1.360
											1.379(4)				
	252	b	0.1818	0.1403	0.1358	0.1472	0.1308	0.1563	0.1308	3	12	1.492(4)	1.508	1.502	1.447
											1.494(4)				
	253	c	0.3636	0.4685	0.4771	0.4671	0.4146	0.3891	0.4146	4	12	1.355(4)	1.342	1.372	1.404
											1.357(4)				
	254	d	0.1818	0.1392	0.1331	0.1503	0.1308	0.1563	0.1308	3	12	1.512(4)	1.505	1.491	1.447
											1.512(4)				
	255	e	0.1818	0.1670	0.1693	0.1546	0.1563	0.1690	0.1563	4	12	1.422(4)	1.427	1.436	1.439
											1.424(4)				
	256	f	0.1818	0.3245	0.3318	0.3288	0.31	0.2459	0.3100	2	13	1.329(4)	1.338	1.402	1.372
											1.331(4)				



303	c	0.5714	0.6703	0.6749	0.6932	0.6224	0.5969	0.6224	3	12	1.343(4)	1.336	1.354	1.377
304	d	0.1429	0.0803	0.0804	0.0780	0.0919	0.1174	0.0919	3	12	1.437(4)	1.452	1.461	1.454
305	e	0.7143	0.8200	0.7987	0.7990	0.8525	0.7834	0.8525	2	14	1.222(4)	1.194	1.220	1.218
306	f	0.1429	0.1195	0.1209	0.1230	0.0403	0.0916	0.1429	3	13	1.379(4)	1.385	1.429	1.382
307	g	0.1429	0.1254	0.1268	0.1287	0.0403	0.0916	0.0403	3	13	1.364(4)	1.363	1.416	1.390
308	h	0.7143	0.7588	0.7560	0.7519	0.8525	0.7834	0.8525	2	14	1.221(4)	1.201	1.229	1.218
309	i	0.1429	0.1158	0.1171	0.1194	0.0660	0.1045	0.0660	4	13	1.386(4)	1.383	1.439	1.381

<sup>a</sup>The nucleobase numeration from Figure 2 and Table 1. The bond length numeration (bn, bl) is according to Figure 2. See the text for the definition of the bond orders  $p_p$ ,  $p_{wkr}$ ,  $p_{wco}$ ,  $p_{wdg}$ ,  $p_{cr}$ ,  $p_m$ ,  $p_s$ , descriptors  $n$  and  $Q$ . Bond lengths: experimental ( $d_{exp}$ ), with esds in parentheses, from HF ( $d_{HF}$ ), PM3 ( $d_{PM3}$ ) and PLS - ( $d_{PLS}$ , model 34) calculations. <sup>b</sup>Experimental bond lengths from nucleoside crystal structures: uncorrected (plain) and corrected (itaics) to libration motion in crystal.



**Table III.** QSPR Data<sup>a</sup> for Nucleobases in Set III

No	bn	bl	$p_p$	$p_{wkr}$	$p_{wco}$	$p_{wdg}$	$p_{cr}$	$p_m$	$p_s$	$n$	$Q$	$d_{exp}$ /Å <sup>b</sup>	$d_{HF}$ /Å	$d_{PM3}$ /Å	$d_{PLS}$ /Å
32	310	a	0.4000	0.4055	0.4054	0.4056	0.4000	0.4000	0.3490	3	12	1.389(3) 1.426	1.409	1.415	1.413
	311	b	0.4000	0.3964	0.3965	0.3964	0.4000	0.4000	0.4510	2	12	1.392(3) 1.426	1.396	1.403	1.411
	312	c	0.4000	0.3974	0.3975	0.3974	0.4000	0.4000	0.4000	2	12	1.389(3) 1.426	1.405	1.413	1.415
	313	d	0.4000	0.4083	0.4082	0.4084	0.4000	0.4000	0.3490	2	12	1.384(3) 1.426	1.394	1.402	1.419
	314	e	0.4000	0.3924	0.3925	0.3923	0.4000	0.4000	0.3490	3	12	1.390(3) 1.426	1.409	1.416	1.413
33	315	a	0.3333	0.3503	0.3537	0.3517	0.4359	0.3846	0.2307	3	13	1.347(1) 1.358(1) 1.351(3)	1.354	1.404	1.359
	316	b	0.3333	0.4531	0.4523	0.4649	0.5385	0.4359	0.5385	2	13	1.323(1) 1.333(1) 1.316(3)	1.290	1.342	1.342
	317	c	0.3333	0.1967	0.1941	0.1834	0.2051	0.2692	0.3333	2	13	1.375(1) 1.389(1) 1.378(3)	1.370	1.398	1.358
	318	d	0.6667	0.8033	0.8051	0.8166	0.7432	0.7049	0.5902	2	12	1.368(1) 1.378(1) 1.360(3)	1.350	1.380	1.379
	319	e	0.3333	0.1967	0.1941	0.1834	0.2307	0.2820	0.2307	3	13	1.369(1) 1.381(1) 1.376(3)	1.375	1.412	1.359
34	320	a	0.4000	0.4340	0.4335	0.4357	0.5026	0.4513	0.2974	3	13	1.242(6)	1.310	1.377	1.349
	321	b	0.4000	0.4313	0.4310	0.4327	0.5282	0.4641	0.5282	2	13	1.243(6)	1.319	1.372	1.337
	322	c	0.4000	0.3370	0.3353	0.3312	0.2718	0.3359	0.4000	2	13	1.349(7)	1.380	1.404	1.347
	323	d	0.4000	0.4618	0.4660	0.4705	0.4765	0.4383	0.3235	2	12	1.376(10)	1.340	1.382	1.421
	324	e	0.4000	0.3358	0.3342	0.3299	0.2974	0.3487	0.2974	3	13	1.349(7)	1.384	1.406	1.349
35	325	a	0.5000	0.5199	0.5197	0.5202	0.5765	0.5383	0.4235	3	12	1.397(1) 1.398(1) 1.399 1.380(3)	1.392	1.398	1.399
	326	b	0.5000	0.4801	0.4803	0.4798	0.4235	0.4617	0.5765	2	12	1.398(1) 1.399(1) 1.399 1.396(3)	1.385	1.389	1.393
	327	c	0.5000	0.5199	0.5197	0.5202	0.5765	0.5383	0.4235	2	12	1.397(1) 1.398(1) 1.399 1.375(3)	1.386	1.392	1.405
	328	d	0.5000	0.4801	0.4803	0.4798	0.4235	0.4617	0.5000	2	12	1.397(1) 1.398(1) 1.399 1.373(3)	1.384	1.389	1.399
	329	e	0.5000	0.5199	0.5197	0.5202	0.5765	0.5383	0.4235	2	12	1.398(1) 1.399(1) 1.399 1.380(3)	1.387	1.392	1.405
36	330	f	0.5000	0.4801	0.4803	0.4798	0.4235	0.4617	0.4235	3	12	1.397(1) 1.398(1) 1.399 1.383(3)	1.389	1.394	1.399
36	331	a	0.5000	0.4965	0.4969	0.4968	0.5000	0.5000	0.4490	3	12	1.337(2) 1.340	1.328	1.367	1.397

	332	b	0.5000	0.5035	0.5031	0.5032	0.5000	0.5000	0.5765	2	12	1.388(2)	1.384	1.396	1.393
	333	c	0.5000	0.4965	0.4969	0.4968	0.5000	0.5000	0.3718	2	13	1.387(2)	1.383	1.398	1.341
	334	d	0.5000	0.5035	0.5031	0.5032	0.5000	0.5000	0.5000	2	13	1.340(2)	1.322	1.351	1.331
	335	e	0.5000	0.4965	0.4969	0.4968	0.5000	0.5000	0.3718	2	13	1.337(2)	1.317	1.359	1.341
	336	f	0.5000	0.5035	0.5031	0.5032	0.5000	0.5000	0.3974	3	13	1.331(2)	1.318	1.352	1.333
<b>37</b>	337	a	0.5000	0.5035	0.5031	0.5032	0.5000	0.5000	0.4490	3	13	1.340(11)	1.346	1.384	1.329
	338	b	0.5000	0.4965	0.4969	0.4968	0.5000	0.5000	0.5765	2	12	1.387(11)	1.364	1.387	1.393
	339	c	0.5000	0.5035	0.5031	0.5032	0.5000	0.5000	0.3718	2	12	1.388(11)	1.395	1.404	1.409
	340	d	0.5000	0.4965	0.4969	0.4968	0.5000	0.5000	0.5000	2	13	1.337(11)	1.320	1.352	1.331
	341	e	0.5000	0.5035	0.5031	0.5032	0.5000	0.5000	0.3718	2	13	1.331(11)	1.306	1.348	1.341
	342	f	0.5000	0.4965	0.4969	0.4968	0.5000	0.5000	0.3974	3	13	1.337(11)	1.337	1.381	1.333
<b>38</b>	343	a	0.2500	0.2010	0.2300	0.2022	0.2245	0.2373	0.2500	4	12	1.510(4)	1.522	1.510	1.426
	344	b	0.2500	0.1364	0.1365	0.1362	0.1990	0.2245	0.1990	3	12	1.500(4)	1.516	1.516	1.437
	345	c	0.7500	0.8636	0.8635	0.8638	0.8265	0.7883	0.8265	2	12	1.328(4)	1.326	1.349	1.354
	346	d	0.2500	0.1364	0.1365	0.1362	0.1990	0.2245	0.1990	3	12	1.474(4)	1.472	1.464	1.437
	347	e	0.2500	0.2773	0.2782	0.2758	0.2755	0.2628	0.2755	4	12	1.393(4)	1.399	1.413	1.424
	348	f	0.2500	0.3853	0.3850	0.3858	0.3010	0.2755	0.1990	3	12	1.380(4)	1.382	1.385	1.437
	349	g	0.7500	0.6147	0.6150	0.6142	0.6735	0.7117	0.7500	2	12	1.393(4)	1.390	1.396	1.360
	350	h	0.2500	0.3853	0.3850	0.3858	0.3265	0.2883	0.2500	2	12	1.373(4)	1.385	1.391	1.439
	351	i	0.7500	0.6147	0.6150	0.6142	0.6735	0.7117	0.7500	2	12	1.400(4)	1.393	1.396	1.360
	352	j	0.2500	0.3853	0.3850	0.3858	0.3010	0.2755	0.1990	3	12	1.377(4)	1.381	1.383	1.437
<b>39</b>	353	a	0.1667	0.1740	0.1739	0.1741	0.1922	0.1922	0.1667	4	12	1.415(5)	1.421	1.422	1.439
	354	b	0.5000	0.5137	0.5135	0.5140	0.5510	0.5255	0.4235	3	12	1.370(5)	1.406	1.416	1.399
	355	c	0.5000	0.4863	0.4865	0.4860	0.4235	0.4617	0.5510	3	12	1.380(5)	1.392	1.397	1.389
	356	d	0.1667	0.1900	0.1898	0.1904	0.2177	0.1922	0.1157	2	12	1.401(5)	1.414	1.422	1.456
	357	e	0.3333	0.3406	0.3402	0.3411	0.3333	0.3333	0.3843	3	12	1.429(5)	1.435	1.443	1.415
	358	f	0.3333	0.2964	0.2961	0.2943	0.2823	0.3078	0.2823	4	12	1.402(5)	1.410	1.401	1.417
	359	g	0.6667	0.7046	0.7039	0.7057	0.7432	0.7049	0.6667	3	12	1.356(5)	1.371	1.379	1.366
	360	h	0.3333	0.2954	0.2961	0.2943	0.2568	0.2950	0.3333	2	12	1.379(5)	1.415	1.410	1.426
	361	i	0.6667	0.7046	0.7039	0.7057	0.7432	0.7049	0.6667	2	12	1.358(5)	1.372	1.378	1.373
	362	j	0.3333	0.2954	0.2961	0.2943	0.2823	0.3078	0.2823	3	12	1.396(5)	1.410	1.404	1.423
<b>40</b>	363	a	0.3750	0.3764	0.3763	0.3760	0.3750	0.3750	0.3750	4	13	1.365(4)	1.365	1.411	1.338
	364	b	0.3750	0.3397	0.3405	0.3389	0.2724	0.3237	0.2724	3	13	1.364(4)	1.375	1.420	1.352
	365	c	0.6250	0.6603	0.6595	0.6611	0.7532	0.6891	0.7532	2	13	1.322(4)	1.279	1.335	1.301
	366	d	0.1250	0.0999	0.0996	0.0983	0.0255	0.0752	0.0255	3	13	1.383(4)	1.384	1.411	1.392
	367	e	0.2500	0.2496	0.2498	0.2489	0.2500	0.25	0.2755	4	12	1.397(4)	1.392	1.419	1.424
	368	f	0.5000	0.5293	0.5306	0.5346	0.5510	0.5255	0.4490	3	12	1.383(4)	1.380	1.407	1.397
	369	g	0.5000	0.4707	0.4698	0.4654	0.3718	0.4359	0.5000	2	13	1.340(4)	1.323	1.341	1.331
	370	h	0.3750	0.3996	0.4500	0.4036	0.5032	0.4391	0.3750	2	13	1.345(4)	1.326	1.381	1.351
	371	i	0.6250	0.6400	0.5995	0.5964	0.5485	0.5867	0.6250	2	13	1.337(4)	1.319	1.343	1.311
	372	j	0.2500	0.2740	0.2743	0.2768	0.3010	0.2755	0.1990	3	13	1.324(4)	1.315	1.373	1.369
<b>41</b>	373	a	0.2857	0.2732	0.2724	0.2720	0.2088	0.2473	0.2857	4	13	1.371(8)	1.333	1.390	1.352
	374	b	0.4286	0.4094	0.4104	0.4081	0.3260	0.3773	0.3260	3	13	1.350(9)	1.388	1.427	1.344
	375	c	0.5714	0.5906	0.5896	0.5919	0.6996	0.6355	0.6996	2	13	1.319(8)	1.278	1.335	1.310
	376	d	0.1429	0.1290	0.1283	0.1264	0.0919	0.1174	0.0919	3	13	1.364(8)	1.373	1.407	1.386

	377	e	0.2857	0.3095	0.3096	0.3112	0.3112	0.2984	0.3112	4	12	1.390(7)	1.417	1.439	1.418
	378	f	0.4286	0.4203	0.4224	0.4236	0.4286	0.4286	0.3776	3	12	1.387(9)	1.355	1.390	1.409
	379	g	0.5714	0.5797	0.5776	0.5764	0.5714	0.5714	0.5714	2	13	1.335(8)	1.355	1.371	1.320
	380	h	0.4286	0.4203	0.4224	0.4236	0.4286	0.4286	0.4286	2	13	1.351(8)	1.348	1.407	1.343
	381	i	0.5714	0.5797	0.5776	0.5764	0.5714	0.5714	0.5714	2	13	1.324(8)	1.292	1.330	1.320
	382	j	0.2857	0.2884	0.2897	0.2903	0.2857	0.2857	0.1831	3	13	1.329(8)	1.327	1.376	1.367
42	383	a	0.2500	0.2680	0.2677	0.2681	0.3269	0.2884	0.2500	4	13	1.370(3)	1.388	1.421	1.358
	384	b	0.2500	0.2075	0.2076	0.2069	0.3526	0.3013	0.1474	3	13	1.382(4)	1.385	1.424	1.373
	385	c	0.7500	0.7925	0.7924	0.7931	0.8265	0.7883	0.8265	2	12	1.377(4)	1.344	1.372	1.354
	386	d	0.2500	0.2075	0.2076	0.2069	0.1990	0.2245	0.1990	3	12	1.429(4)	1.441	1.442	1.437
	387	e	0.2500	0.2792	0.2793	0.2807	0.2755	0.2628	0.2755	4	12	1.423(4)	1.401	1.420	1.424
	388	f	0.2500	0.2453	0.2455	0.2444	0.2500	0.2500	0.1990	3	12	1.405(4)	1.398	1.398	1.437
	389	g	0.7500	0.7547	0.7445	0.7556	0.7500	0.7500	0.7500	2	12	1.387(5)	1.375	1.382	1.360
	390	h	0.2500	0.2453	0.2455	0.2444	0.2500	0.2500	0.2500	2	12	1.425(5)	1.402	1.407	1.439
	391	i	0.7500	0.7547	0.7545	0.7556	0.7500	0.7500	0.7500	2	12	1.385(5)	1.377	1.382	1.360
	392	j	0.2500	0.2453	0.2455	0.2444	0.2500	0.2500	0.1990	3	12	1.401(4)	1.397	1.401	1.437
43	393	a	0.3333	0.2900	0.2905	0.2891	0.3078	0.3206	0.3333	4	12	1.419(2)	1.438	1.432	1.413
												1.424(2)			
												1.405(13)			
	394	b	0.6667	0.7100	0.7095	0.7109	0.7177	0.6922	0.7177	3	12	1.373(2)	1.362	1.374	1.362
												1.380(2)			
												1.388(18)			
	395	c	0.3333	0.2900	0.2905	0.2891	0.2568	0.2950	0.3333	2	12	1.407(2)	1.417	1.412	1.426
												1.413(2)			
												1.349(13)			
	396	d	0.6667	0.7100	0.7095	0.7109	0.7432	0.7049	0.7431	2	12	1.368(2)	1.354	1.367	1.367
												1.373(2)			
												1.336(13)			
	397	e	0.3333	0.2900	0.2905	0.2891	0.2823	0.3078	0.2823	3	12	1.424(2)	1.422	1.420	1.423
												1.431(2)			
												1.408(18)			
	398	f	0.3333	0.4201	0.4190	0.4219	0.3588	0.3460	0.3588	4	12	1.420(2)	1.412	1.414	1.411
												1.426(2)			
												1.398(13)			
	399	g	0.3333	0.2900	0.2905	0.2891	0.2823	0.3078	0.2823	3	12	1.419(2)	1.419	1.422	1.423
												1.424(2)			
												1.422(13)			
	400	h	0.6667	0.7100	0.7095	0.7109	0.7177	0.6922	0.6667	2	12	1.373(2)	1.358	1.368	1.373
												1.380(2)			
												1.371(18)			
	401	i	0.3333	0.2900	0.2905	0.2891	0.2568	0.2950	0.3333	2	12	1.407(2)	1.413	1.414	1.426
												1.413(2)			
												1.407(13)			
	402	j	0.6667	0.7100	0.7095	0.7109	0.7177	0.6922	0.6667	2	12	1.368(2)	1.360	1.367	1.373
												1.373(2)			
												1.363(18)			
	403	k	0.3333	0.2900	0.2905	0.2891	0.2823	0.3078	0.2823	3	12	1.424(2)	1.423	1.422	1.423
												1.431(2)			
												1.453(18)			
44	404	a	0.5000	0.5068	0.5052	0.5045	0.5000	0.5000	0.4490	3	12	1.370(3)	1.393	1.401	1.397
	405	b	0.5000	0.4932	0.4948	0.4955	0.5000	0.5000	0.5765	2	12	1.358(3)	1.390	1.394	1.393
	406	c	0.5000	0.5068	0.5052	0.5045	0.5000	0.5000	0.4235	2	12	1.356(3)	1.371	1.392	1.405
	407	d	0.5000	0.4932	0.4948	0.4955	0.5000	0.5000	0.5000	2	13	1.341(3)	1.337	1.370	1.331
	408	e	0.5000	0.5068	0.5052	0.5045	0.5000	0.5000	0.3718	2	13	1.327(3)	1.338	1.368	1.341
	409	f	0.5000	0.4932	0.4948	0.4955	0.5000	0.5000	0.4490	3	12	1.360(3)	1.377	1.397	1.397
45	410	a	0.5000	0.5154	0.5156	0.5045	0.5510	0.5255	0.4490	3	12	1.338(3)	1.391	1.399	1.397
												1.362(5)			
	411	b	0.5000	0.4846	0.4844	0.4955	0.4235	0.4617	0.5765	2	12	1.382(3)	1.381	1.389	1.393
												1.392(6)			
	412	c	0.5000	0.5154	0.5156	0.5045	0.5765	0.5383	0.4235	2	12	1.366(3)	1.386	1.396	1.405
												1.359(6)			
	413	d	0.5000	0.4846	0.4844	0.4955	0.3718	0.4359	0.5000	2	13	1.374(3)	1.318	1.351	1.331

													<b>1.321(6)</b>		
	414	e	0.5000	0.5154	0.5156	0.5045	0.6282	0.5641	0.3718	2	13	1.380(3)	1.323	1.353	1.341
												<b>1.341(5)</b>			
	415	f	0.5000	0.4846	0.4844	0.4955	0.4490	0.4745	0.4490	3	12	1.338(3)	1.387	1.397	1.397
												<b>1.362(5)</b>			
46	416	a	0.1667	0.1803	0.1784	0.1785	0.2436	0.2052	0.1667	4	13	1.372(3)	1.382	1.421	1.371
	417	b	0.5000	0.4374	0.4424	0.4415	0.3974	0.4487	0.3974	3	13	1.361(3)	1.371	1.417	1.333
	418	c	0.5000	0.5626	0.5576	0.5585	0.6282	0.5641	0.6282	2	13	1.305(3)	1.280	1.331	1.321
	419	d	0.1667	0.1355	0.1368	0.1377	0.0641	0.1154	0.0641	3	13	1.396(3)	1.384	1.418	1.386
	420	e	0.3333	0.3530	0.3534	0.3539	0.3588	0.3460	0.3588	4	12	1.410(3)	1.394	1.417	1.411
	421	f	0.3333	0.3312	0.3314	0.3299	0.3333	0.3333	0.2823	3	12	1.380(3)	1.392	1.399	1.423
	422	g	0.6667	0.6688	0.6686	0.6701	0.6667	0.6667	0.6667	2	12	1.388(3)	1.378	1.383	1.373
	423	h	0.3333	0.3312	0.3314	0.3299	0.3333	0.3333	0.3333	2	12	1.405(4)	1.405	1.407	1.426
	424	i	0.6667	0.6688	0.6686	0.6701	0.6667	0.6667	0.6667	2	12	1.368(3)	1.377	1.383	1.373
	425	j	0.3333	0.3312	0.3314	0.3299	0.3333	0.3333	0.2823	3	12	1.395(3)	1.394	1.399	1.423
47	426	a	0.1667	0.1684	0.1678	0.1680	0.1667	0.1667	0.1667	4	13	1.373(3)	1.404	1.423	1.371
	427	b	0.5000	0.4866	0.4876	0.4878	0.3974	0.4487	0.3974	3	13	1.332(4)	1.310	1.377	1.333
	428	c	0.5000	0.5134	0.5124	0.5122	0.6282	0.5641	0.6282	2	13	1.322(3)	1.316	1.371	1.321
	429	d	0.1667	0.1552	0.1552	0.1564	0.0641	0.1154	0.0641	3	13	1.389(3)	1.395	1.417	1.386
	430	e	0.3333	0.3743	0.3750	0.3770	0.3588	0.3460	0.3588	4	12	1.398(3)	1.381	1.416	1.411
	431	f	0.3333	0.3021	0.3019	0.2986	0.2823	0.3078	0.2823	3	12	1.366(3)	1.391	1.402	1.423
	432	g	0.6667	0.6979	0.6981	0.7014	0.7432	0.7049	0.6667	2	12	1.373(4)	1.379	1.382	1.373
	433	h	0.3333	0.3021	0.3019	0.2986	0.2568	0.2950	0.3333	2	12	1.413(4)	1.404	1.411	1.426
	434	i	0.6667	0.6979	0.6981	0.7014	0.7432	0.7049	0.6667	2	12	1.344(4)	1.378	1.382	1.373
	435	j	0.3333	0.3021	0.3019	0.2986	0.2823	0.3078	0.2823	3	12	1.391(4)	1.393	1.402	1.423
48	436	a	0.5000	0.8653	0.8608	0.8620	0.5510	0.5255	0.4490	3	12	1.334(3)	1.324	1.344	1.397
	437	b	0.1667	0.0346	0.0358	0.0355	0.1157	0.1412	0.2177	3	12	1.471(3)	1.492	1.487	1.442
	438	c	0.5000	0.8653	0.8608	0.8620	0.6382	0.5691	0.3618	2	14	1.223(3)	1.191	1.215	1.274
	439	d	0.3333	0.1100	0.1034	0.1025	0.2823	0.3078	0.2823	3	12	1.477(3)	1.493	1.488	1.423
	440	e	0.3333	0.7989	0.7922	0.7939	0.4098	0.3716	0.3333	2	12	1.334(3)	1.321	1.335	1.426
	441	f	0.1667	0.0664	0.0686	0.0680	0.1157	0.1412	0.1157	3	12	1.471(3)	1.491	1.492	1.450
	442	g	0.3333	0.7989	0.7922	0.7939	0.4715	0.4024	0.4715	2	14	1.223(3)	1.201	1.216	1.279
	443	h	0.5000	0.1347	0.1392	0.1380	0.4745	0.4873	0.4745	4	12	1.477(3)	1.504	1.497	1.388
49	444	a	0.5000	0.8537	0.8491	0.8493	0.5510	0.5255	0.4490	3	12	1.336(2)	1.333	1.348	1.397
	445	b	0.2500	0.0620	0.0638	0.0628	0.1735	0.2118	0.3265	2	12	1.445(4)	1.480	1.454	1.433
	446	c	0.5000	0.8537	0.8491	0.8493	0.5765	0.5383	0.4490	2	12	1.336(2)	1.341	1.341	1.403
	447	d	0.2500	0.0843	0.0871	0.0879	0.1990	0.2245	0.2500	3	12	1.463(2)	1.473	1.483	1.433
	448	e	0.7500	0.9157	0.9129	0.9121	0.8882	0.8191	0.7500	2	14	1.215(2)	1.183	1.212	1.224
	449	f	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	4	12	1.541(3)	1.550	1.532	1.466
	450	g	0.5000	0.8537	0.8491	0.8493	0.6382	0.5691	0.5000	2	14	1.215(2)	1.192	1.212	1.263
	451	h	0.5000	0.1463	0.1509	0.1507	0.4745	0.4873	0.4745	4	12	1.463(2)	1.488	1.490	1.388
50	452	a	0.1111	0.0809	0.0811	0.0816	0.0856	0.0984	0.1111	4	12	1.485(4)	1.499	1.497	1.448
	453	b	0.6667	0.7309	0.7291	0.7249	0.8049	0.7358	0.6667	2	14	1.202(3)	1.185	1.213	1.237
	454	c	0.2222	0.1882	0.1898	0.1934	0.1196	0.1709	0.1196	3	13	1.388(3)	1.382	1.444	1.377
	455	d	0.2222	0.2087	0.2101	0.2133	0.1196	0.1709	0.3248	3	13	1.376(3)	1.384	1.443	1.361
	456	e	0.5556	0.6160	0.6146	0.6101	0.6938	0.6247	0.5556	2	14	1.218(3)	1.187	1.221	1.254
	457	f	0.2222	0.1752	0.1754	0.1766	0.1967	0.2095	0.1967	4	12	1.478(4)	1.494	1.490	1.433
	458	g	0.3333	0.3498	0.3497	0.3472	0.3588	0.3461	0.3588	4	12	1.389(4)	1.358	1.419	1.411
	459	h	0.4444	0.4749	0.4749	0.4763	0.3934	0.4189	0.3934	3	12	1.374(4)	1.377	1.377	1.406
	460	i	0.4444	0.4366	0.4366	0.4345	0.4444	0.4444	0.4444	2	12	1.385(4)	1.387	1.401	1.408
	461	j	0.4444	0.4825	0.4825	0.4838	0.5209	0.4827	0.4444	2	12	1.377(4)	1.391	1.383	1.408
	462	k	0.4444	0.4308	0.4308	0.4288	0.3934	0.4189	0.4444	3	12	1.382(4)	1.394	1.412	1.402
	463	l	0.5556	0.5692	0.5692	0.5712	0.5811	0.5684	0.5301	4	12	1.373(4)	1.388	1.385	1.380

<sup>a</sup>The nucleobase numeration from Figure 2 and Table 1. The bond length numeration (bn, bl) is according to Figure 2. See the text for the definition of the bond orders  $p_p$ ,  $p_{wkr}$ ,  $p_{wco}$ ,  $p_{wdg}$ ,  $p_{ct}$ ,  $p_m$ ,  $p_s$ , descriptors  $n$  and  $Q$ . Bond lengths: experimental ( $d_{exp}$ ), with esds in parentheses, from HF ( $d_{HF}$ ), PM3 ( $d_{PM3}$ ) and PLS - ( $d_{PLS}$ , model 34) calculations. <sup>b</sup>Experimental bond lengths: from nucleobase crystal structures - uncorrected (plain) and corrected (italics) to libration motion in crystal; from gas-phase nucleobase structure (plain, without esd); from nucleoside crystal structure, uncorrected to libration motion (bold).