Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Complete conformational space of the potential HIV-1 reverse transcriptase inhibitors d4U and d4C. A quantum chemical study

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Table S1. Statistical parameters corresponding to the sugar ring and glycoside bond of d4U

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Cartesian coordinates of the 20 d4U structures

Cartesian coordinates of the 19 d4C structures

Table S1. Statistical parameters corresponding to the sugar ring and glycoside bond of d4U, calculated at the B3LYP/6-31++G(d,p) level of theory[a]

Deviations from the C1'O4'C4' plane (in Å)

	C2'	C3'
min	0.039	-0.007
max	0.254	0.239
mean	0.156	0.135

Bond lengths (in Å)

	O4'C1'	C1'C2'	C2'C3'	C3'C4'	C4'O4'	C2'N1
min	1.412	1.507	1.330	1.502	1.439	1.469
max	1.433	1.510	1.333	1.508	1.455	1.483
mean	1.423	1.508	1.332	1.505	1.445	1.476
std	0.007	0.001	0.001	0.002	0.005	0.005

Bond angles (in degrees)

	O4'C1'C2'	C1'C2'C3'	C2'C3'C4'	C3'C4'O4'	C4'O4'O1'
min	104.5	109.2	109.9	103.8	110.3
max	105.5	109.9	110.4	104.4	111.0
mean	105.0	109.6	110.2	104.2	110.6
std	0.4	0.2	0.2	0.2	0.1
std/mean	0.004	0.002	0.002	0.002	0.001

[a] Min, max, mean, std: minimum, maximum, mean and standard deviation values.

Table S2. Statistical parameters corresponding to the sugar ring and glycoside bond of d4C, calculated at the B3LYP/6-31++G(d,p) level of theory[a]

Deviations from the C1'O4'C4' plane (in Å)

	C2'	C3'
min	-0.025	-0.042
max	0.285	0.280
mean	0.109	0.087

Bond lengths (in Å)

	O4'C1'	C1'C2'	C2'C3'	C3'C4'	C4'O4'	C2'N1
min	1.413	1.506	1.330	1.503	1.439	1.474
max	1.429	1.509	1.333	1.508	1.454	1.494
mean	1.419	1.508	1.331	1.504	1.447	1.484
std	0.003	0.001	0.001	0.002	0.004	0.006

Bond angles (in degrees)

	O4'C1'C2'	C1'C2'C3'	C2'C3'C4'	C3'C4'O4'	C4'O4'O1'
min	104.6	109.3	109.9	103.7	110.2
max	105.3	110.0	110.5	104.4	110.9
mean	105.1	109.5	110.2	104.2	110.6
std	0.2	0.2	0.1	0.2	0.2
std/mean	0.002	0.002	0.001	0.002	0.002

[a] min, max, mean, std: minimum, maximum, mean and standard deviation values.

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Table S3. Geometric, energetic and electron-topological characteristics of the specific intramolecular contacts in the d4U conformers

	conformer (χ/γ/β)	H-bond	d(A···B)[a]	d(H···B)[b]	∠AHB[c]	ρ[d]	$\nabla^2\rho$[e]	100·ε[f]	E_{HB}[g]	d(BCP-RCP)[h]	C_{ij}[i]
1	high-anti/g^+/g^+	C6H···O5'	3.438	2.669	127.5	0.007	0.025	32	1.30	0.719	29.443
		C1'H···O2	2.782	2.238	108.3	0.019	0.078	130	4.60	0.192	3.257
2	high-anti/g^+/t	C6H···O5'	3.308	2.263	161.0	0.014	0.043	8	3.31	0.867	10.978
		C1'H···O2	2.788	2.225	109.5	0.019	0.077	100	4.68	0.227	3.100
3	high-anti/t/g^-	C1'H···O2	2.786	2.224	109.4	0.019	0.078	103	4.69	0.221	3.119
		C5'H1···HC6	3.446	2.576	136.7	0.003	0.012	81	0.44	0.223	42.066
4	high-anti/g^-/t	C1'H···O2	2.789	2.230	109.3	0.019	0.077	109	4.64	0.216	3.161
		C5'H2···HC6	3.490	2.627	136.1	0.003	0.011	405	0.42	0.062	56.529
5	anti/g^+/g^-	C6H···O5'	3.311	2.233	172.0	0.016	0.044	6	3.63	0.833	9.339
		C1'H···O2	2.769	2.248	106.7	0.019	0.079	154	4.60	0.169	3.932
6	syn/g^+/g^+	O5'H···O2	2.851	1.888	169.2	0.026	0.084	4	6.10	1.052	5.697
7	high-anti/g^-/g^-	C1'H···O2	2.787	2.227	109.3	0.019	0.077	106	4.66	0.219	3.150
8	syn/t/g^-	C5'H1···O2	3.422	2.542	136.6	0.008	0.029	10	1.70	0.780	25.673
9	anti/g^+/g^+	C6H···O4'	2.706	2.234	103.9	0.019	0.076	55	4.62	0.650	3.456
10	anti/t/t	C6H···O4'	2.715	2.243	104.0	0.019	0.076	64	4.60	0.614	3.827
11	high-anti/g^-/g^+	C1'H···O2	2.788	2.224	109.6	0.019	0.077	100	4.68	0.226	3.113
		C5'H2···HC6	3.502	2.612	139.0	0.003	0.011	264	0.42	0.090	55.110
12	anti/t/g^+	C6H···O4'	2.720	2.556	103.5	0.018	0.075	72	4.51	0.576	3.810
13	high-anti/t/t	C1'H···O2	2.792	2.227	109.6	0.019	0.077	103	4.65	0.223	3.102
14	syn/g^-/t	C5'H2···O2	3.374	2.506	135.3	0.009	0.030	10	1.85	0.814	24.578
15	anti/g^-/g^+	C6H···O4'	2.737	2.282	103.0	0.018	0.072	78	4.30	0.541	5.574
16	high-anti/t/g^+	C1'H···O2	2.788	2.221	109.8	0.019	0.077	96	4.70	0.233	3.079
17	syn/t/t	C5'H1···O2	3.355	2.464	137.6	0.010	0.032	11	2.04	0.802	25.498
18	syn/g^-/g^+	C5'H2···O2	3.374	2.484	137.7	0.009	0.032	10	1.96	0.828	22.929
		C2···O2	2.907	-	-	0.012	0.043	250	2.66	0.145	5.412
19	syn/g^-/g^-	C5'H2···O2	3.378	2.537	133.1	0.008	0.029	10	1.68	0.792	26.736
20	syn/t/g^+	C5'H1···O2	3.389	2.504	137.4	0.009	0.030	11	1.82	0.806	26.595
		C2'···O2	2.896	-		0.012	0.044	213	2.70	0.164	5.548
		Minimal value:	2.706	1.888	103.0	0.003	0.011	4	0.42	0.062	3.079
		Maximal value:	3.502	2.669	172.0	0.026	0.084	405	6.1	1.052	56.529

[a] Distance between the donor (A) and acceptor (B) atoms (in Å); [b] Distance between the hydrogen (H) and B atom (in Å); [c] H-bond angle (for putative H-bonds) (in degrees); [d] Electron density value at the BCP (in a.u.); [e] Laplacian of the electron density at the BCP (in a.u.); [f] Ellipticity at the BCP; [g] Energy of interaction, calculated by formula (2) (in kcal/mol); [h] Distance from the BCP to the nearest ring critical point (RCP, the so-called (3,+1) point) (in a.u.). [i] Compliance constant (inÅ/mDyn)

Table S4. Geometric, energetic and electron-topological characteristics of the specific intramolecular contacts in the d4C conformers

	conformer (χ/γ/β)	H-bond	d(A···B)[a]	d(H···B)[b]	∠AHB[c]	ρ[d]	$\nabla^2\rho$[e]	100·ε[f]	E_{HB}[g]	d(BCP-RCP)[h]	C_{ij}[i]
1	high-anti/g^+/g^+	C6H···O5'	3.445	2.672	127.7	0.007	0.025	41	1.29	1.321	31.830
		C1'H···O2	2.748	2.182	109.5	0.021	0.080	55	5.09	0.599	3.191
2	high-anti/g^-/t	C1'H···O2	2.754	2.175	110.4	0.021	0.080	49	5.15	0.622	3.066
		C5'H1···HC6	3.513	2.562	146.0	0.004	0.012	181	0.46	0.244	50.329
3	anti/g^+/g^-	C6H···O5'	3.333	2.383	145.5	0.012	0.037	5	2.65	0.696	20.378
4	anti/t/g^-	C6H···O4'	2.748	2.336	100.5	0.016	0.070	176	4.04	0.168	5.647
5	syn/g^+/g^+	O5'H···O2	2.803	1.836	170.0	0.029	0.096	4	6.80	1.081	4.920
6	high-anti/t/g^-	C1'H···O2	2.750	2.169	110.5	0.022	0.080	48	5.21	0.632	3.071
		C5'H2···HC6	3.452	2.504	145.4	0.004	0.013	62	0.51	0.513	51.569
7	high-anti/g^+/t	C6H···O5'	3.326	2.253	169.4	0.015	0.043	7	3.38	0.828	10.656
		C1'H···O2	2.739	2.198	107.9	0.021	0.080	62	5.01	0.295	4.206
8	anti/g^+/g^+	C6H···O4'	2.697	2.244	102.7	0.019	0.077	65	4.58	0.317	3.429
9	anti/g^-/t	C6H···O4'	2.719	2.281	101.9	0.018	0.073	90	4.36	0.267	4.671
10	high-anti/g^-/g^-	C1'H···O2	2.752	2.172	110.4	0.021	0.080	49	5.17	0.627	3.048
11	anti/g^-/g^-	C6H···O4'	2.723	2.290	101.6	0.018	0.073	99	4.30	0.251	4.767
12	anti/t/g^+	C6H···O4'	2.705	2.255	102.5	0.019	0.077	81	4.57	0.288	3.631
13	syn/t/g^-	C5H1···O2	3.361	2.478	136.8	0.009	0.032	11	1.98	0.804	22.315
		C2···O2	2.868	-	-	0.013	0.046	226	2.88	0.171	5.871
14	anti/t/t	C6H···O4'	2.702	2.247	102.9	0.019	0.077	73	4.61	0.304	3.666
15	anti/g^-/g^+	C6H···O4'	2.716	2.272	102.3	0.018	0.074	83	4.42	0.281	4.039
16	syn/g^-/t	C5'H2···O2	3.297	2.423	135.9	0.010	0.035	10	2.25	0.851	19.585
		C2···O2	2.883	-	-	0.013	0.045	232	2.82	0.164	5.496
17	syn/g^-/g^+	C5'H2···O2	3.306	2.407	138.5	0.011	0.036	10	2.35	0.859	18.475
		C2'···O2	2.858	-	-	0.014	0.046	126	2.92	0.250	5.119
18	syn/g-/g-	C5H2···O2	3.318	2.480	132.7	0.009	0.032	11	1.94	0.814	22.989
		C2'···O2	2.878	-	-	0.013	0.046	264	2.85	0.150	5.808
19	syn/t/g^+	C5H1···O2	3.345	2.462	137.0	0.010	0.033	12	2.03	0.825	23.680
		C2'···O2	2.839	-	-	0.014	0.047	105	3.00	0.280	5.382
		Minimal value:	2.697	1.836	100.5	0.004	0.012	4	0.46	0.164	3.048
		Maximal value:	3.513	2.562	170.0	0.029	0.096	264	6.80	1.321	51.569

[a] Distance between the donor (A) and acceptor (B) atoms (in Å); [b] Distance between the hydrogen (H) and B atom (in Å); [c] H-bond angle (for putative H-bonds) (in degrees); [d] Electron density value at the BCP (in a.u.); [e] Laplacian of the electron density at the BCP (in a.u.); [f] Ellipticity at the BCP; [g] Energy of interaction, calculated by formula (2) (in kcal/mol); [h] Distance from the BCP to the nearest ring critical point (RCP, the so-called (3,+1) point) (in a.u.). [i] Compliance constant (inÅ/mDyn)

Table S5. NBO analysis of donor-acceptor interactions in d4U through specific intramolecular contacts[a]

	conformer (χ/γ/β)	H-bond	donor–acceptor NBOs	E(2)	Occupancy of LP	Energy of LP	Occupancy of BD*	Energyof BD*
1	high-anti/g^+/g^+	C6H···O5'	$LP(2)_{O5'} - BD^*(1)_{C6H}$	0.58	1.952	-0.322	0.017	0.451
		C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.62	1.840	-0.273	0.034	0.434
2	high-anti/g^+/t	C6H···O5'	$LP(2)_{O5'} - BD^*(1)_{C6H}$	2.72	1.960	-0.354	0.022	0.478
		C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.79	1.842	-0.266	0.034	0.441
3	high-anti/t/g^-	C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.80	1.839	-0.276	0.035	0.431
		C5'H1···HC6	–	–	–	–	–	–
4	high-anti/g^-/t	C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.75	1.840	-0.271	0.035	0.437
		C5'H2···HC6	–	–	–	–	–	–
5	anti/g^+/g^-	C6H···O5'	$LP(2)_{O5'} - BD^*(1)_{C6H}$	3.82	1.950	-0.335	0.026	0.479
			$LP(1)_{O2}$– $BD^*(1)_{C6H}$	1.58	1.979	-0.626		
		C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.40	1.845	-0.268	0.034	0.434
6	syn/g^+/g^+	O5'H···O2	$LP(1)_{O2} - BD^*(1)_{O5'H'}$	10.25	1.965	-0.722	0.028	0.501
			$LP(2)_{O2} - BD^*(1)_{O5'H'}$		1.850	-0.288		
7	high-anti/g^-/g^-	C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.77	1.840	-0.272	0.035	0.434
8	syn/t/g^-	C5'H1···O2	$LP(1)_{O2} - BD^*(1)_{C5'H1'}$	0.61	1.976	-0.718	0.025	0.444
9	anti/g^+/g^+	C6H···O4'	$LP(1)_{O4'} - BD^*(1)_{C6H}$	1.37	1.965	-0.600	0.018	0.445
			$LP(2)_{O4'} - BD^*(1)_{C6H}$		1.914	-0.348		
10	anti/t/t	C6H···O4'	$LP(2)_{O4'} - BD^*(1)_{C6H}$	0.96	1.906	-0.333	0.017	0.461
11	high-anti/g^-/g^+	C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.81	1.839	-0.274	0.035	0.432
		C5'H2···HC6	–	–	–	–	–	–
12	anti/t/g^+	C6H···O4'	$LP(2)_{O4'} - BD^*(1)_{C6'H'}$	0.91	1.906	-0.335	0.017	0.464
13	high-anti/t/t	C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.79	1.840	-0.271	0.035	0.436
14	syn/g^-/t	C5'H2···O2	$LP(1)_{O2} - BD^*(1)_{C5'H2'}$	0.72	1.976	-0.714	0.022	0.447
15	anti/g^-/g^+	C6H···O4'	$LP(2)_{O4'} - BD^*(1)_{C6'H'}$	0.90	1.909	-0.342	0.018	0.452
16	high-anti/t/g^+	C1'H···O2	$LP(2)_{O2} - BD^*(1)_{C1'H'}$	1.84	1.840	-0.272	0.035	0.433
17	syn/t/t	C5'H1···O2	$LP(1)_{O2} - BD^*(1)_{C5'H1'}$	0.76	1.976	-0.715	0.022	0.446
18	syn/g^-/g^+	C5'H2···O2	$LP(1)_{O2} - BD^*(1)_{C5'H2'}$	0.75	1.976	-0.717	0.019	0.444
19	syn/g^-/g^-	C5'H2···O2	$LP(1)_{O2} - BD^*(1)_{C5'H2'}$	0.63	1.976	-0.713	0.018	0.457
20	syn/t/g^+	C5'H1···O2	$LP(1)_{O2} - BD^*(1)_{C5'H1'}$	0.62	1.976	-0.714	0.036	0.402

[a] LP: orbital that corresponds to the electron lone pair; BD^*: antibonding orbital; $E^{(2:}$ stabilization energy, defined by formula (3), in kcal/mol. Note that NBO does not give donor-acceptor interactions for H···H contacts.

Table S6. NBO analysis of donor-acceptor interactions in d4C through specific intramolecular contacts[a]

conformer (χ/γ/β)		H-bond	donor–acceptor NBOs	E(2)	Occupancy of LP	Energy of LP	Occupancy of BD*	Energy of BD*
1	high-anti/g^+/g^+	C6H···O5'	$LP(2)_{O5'} - BD^*_{C6H}$	0.57	1.953	-0.314	0.018	0.455
		C1'H···O2	$LP(1)_{O2} - BD^*_{C1'H'}$	2.71	1.976	-0.675	0.036	0.452
			$LP(2)_{O2} - BD^*_{C1'H'}$		1.844	-0.233		
2	high-anti/g^-/t	C1'H···O2	$LP(1)_{O2} - BD^*_{C1'H'}$	2.85	1.976	-0.674	0.037	0.455
			$LP(2)_{O2} - BD^*_{C1'H'}$		1.845	-0.232		
		C5'H1···HC6	–	–	–	–	–	–
3	anti/g^+/g^-	C6H···O5'	$LP(2)_{O5'} - BD^*_{C6H}$	1.89	1.952	-0.322	0.022	0.480
4	anti/t/g^-	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.72	1.916	-0.335	0.018	0.453
5	syn/g^+/g^+	O5'H···O2	$LP(2)_{O2} - BD^*_{O5'H'}$	12.50	1.857	-0.249	0.034	0.518
			$LP(1)_{O2} - BD^*_{O5'H'}$		1.960	-0.680		
6	high-anti/t/g^-	C1'H···O2	$LP(1)_{O2} - BD^*_{C1'H'}$	2.94	1.976	-0.678	0.037	0.449
			$LP(2)_{O2} - BD^*_{C1'H'}$		1.844	-0.236		
		C5'H2···HC6	–	–	–	–	–	–
7	high-anti/g^+/t	C6H···O5'	$LP(2)_{O5'} - BD^*_{C6H}$	1.81	1.959	-0.350	0.024	0.487
			$LP(1)_{O5'} - BD^*_{C6H}$		1.978	-0.607		
		C1'H···O2	$LP(2)_{O2} - BD^*_{C1'H'}$	3.20	1.850	-0.226	0.035	0.458
8	anti/g^+/g^+	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.77	1.916	-0.336	0.018	0.449
			$LP(1)_{O4'} - BD^*_{C6H}$	0.52	1.966	-0.589		
9	anti/g-/t	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.88	1.913	-0.327	0.018	0.458
10	high-anti/g^-/g^-	C1'H···O2	$LP(2)_{O2} - BD^*_{C1'H'}$	2.89	1.976	-0.675	1.844	-0.233
11	anti/g^-/g^-	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.84	1.912	-0.329	0.018	0.458
12	anti/t/g^+	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.88	1.908	-0.323	0.018	0.468
13	syn/t/g^-	C5′H1···O2	$LP(1)_{O2} - BD^*_{C5'H1'}$	0.83	1.975	-0.678	0.025	0.465
14	anti/t/t	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.92	1.909	-0.320	0.018	0.465
15	anti/g^-/g^+	C6H···O4'	$LP(2)_{O4'} - BD^*_{C6H}$	0.88	1.911	-0.329	0.018	0.457
16	syn/g^-/t	C5'H2···O2	$LP(1)_{O2} - BD^*_{C5'H2'}$	1.06	1.975	-0.674	0.021	0.467
17	syn/g^-/g^+	C5'H2···O2	$LP(1)_{O2} - BD^*_{C5'H2'}$	1.05	1.975	-0.678	0.020	0.466
18	syn/g^-/g^-	C5H2···O2	$LP(1)_{O2} - BD^*_{C5'H2'}$	0.83	1.975	-0.673	0.018	0.477
19	syn/t/g^+	C5H1···O2	$LP(1)_{O2} - BD^*_{C5'H1'}$	0.73	1.975	-0.674	0.019	0.476

[a] LP: orbital that corresponds to the electron lone pair; BD^*: antibonding orbital; $E^{(2:}$ stabilization energy, defined by formula (3), in kcal/mol. Note that NBO does not give donor-acceptor interactions for H···H contacts.

Cartesian coordinates of the 20 d4U structures optimised with B3LYP/6-31++G(d,p)

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25
d4U 1
C       -0.759296000     -1.190370000      0.189933000
C       -1.565610000     -1.006066000      1.450005000
C       -2.760230000     -0.499213000      1.151294000
C       -2.888312000     -0.309725000     -0.336814000
O       -1.581234000     -0.643853000     -0.848430000
H       -0.528233000     -2.235308000     -0.033798000
H       -1.189051000     -1.282917000      2.427798000
H       -3.561499000     -0.274746000      1.846390000
H       -3.621031000     -1.023407000     -0.749813000
C       -3.283884000      1.089521000     -0.819403000
H       -4.248129000      1.362552000     -0.377900000
H       -3.407115000      1.065343000     -1.910421000
O       -2.355725000      2.092893000     -0.434794000
H       -1.556051000      1.967768000     -0.963588000
N        0.545289000     -0.514432000      0.214007000
N        2.816543000     -0.454221000     -0.339210000
C        1.652461000     -1.200018000     -0.314498000
C        0.647831000      0.800912000      0.629100000
C        1.800942000      1.504354000      0.581634000
C        3.011516000      0.881043000      0.066859000
H       -0.276180000      1.231381000      0.998945000
O        4.114575000      1.401080000     -0.029685000
O        1.602360000     -2.355920000     -0.707211000
H        3.627893000     -0.935771000     -0.711149000
H        1.854260000      2.529463000      0.922246000
25
d4U 2
C       -0.713243000     -1.223144000      0.003536000
C       -1.498832000     -1.181430000      1.290376000
C       -2.711893000     -0.681816000      1.065068000
C       -2.867056000     -0.345381000     -0.395555000
O       -1.574626000     -0.627492000     -0.965616000
H       -0.439681000     -2.236419000     -0.302120000
H       -1.091158000     -1.532448000      2.230985000
H       -3.500131000     -0.531960000      1.793753000
H       -3.602687000     -1.011551000     -0.875224000
C       -3.303716000      1.082992000     -0.705184000
H       -4.371464000      1.178974000     -0.456805000
H       -3.177979000      1.254356000     -1.781866000
O       -2.524844000      2.003312000      0.058769000
H       -2.677940000      2.897523000     -0.270413000
N        0.564588000     -0.491464000      0.058254000
N        2.884597000     -0.415721000     -0.187062000
C        1.744908000     -1.197740000     -0.209221000
C        0.573610000      0.869822000      0.297568000
C        1.709717000      1.603685000      0.312950000
C        2.992196000      0.968047000      0.060395000
H       -0.406456000      1.309327000      0.449824000
O        4.089290000      1.511984000      0.046057000
O        1.775923000     -2.401045000     -0.431271000
H        3.750286000     -0.910033000     -0.372254000
H        1.692820000      2.668246000      0.502659000
25
d4U 3
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C         0.666491000      1.165927000      0.057032000
C         1.361488000      1.340808000      1.384129000
C         2.586850000      0.818955000      1.328057000
C         2.838627000      0.232404000     -0.034526000
O         1.574465000      0.382641000     -0.722568000
H         0.455643000      2.112538000     -0.448215000
H         0.900014000      1.855468000      2.218956000
H         3.328985000      0.824923000      2.118710000
H         3.595364000      0.809246000     -0.587621000
C         3.247277000     -1.240257000     -0.055967000
H         2.498606000     -1.835696000      0.488631000
H         4.212116000     -1.360300000      0.447711000
O         3.422446000     -1.719270000     -1.378493000
H         2.596703000     -1.571523000     -1.861732000
N        -0.637303000      0.491831000      0.142377000
N        -2.884268000      0.313034000     -0.477449000
C        -1.724696000      1.063234000     -0.540142000
C        -0.752830000     -0.730287000      0.776128000
C        -1.900071000     -1.442302000      0.814117000
C        -3.091897000     -0.930154000      0.152924000
H         0.156742000     -1.079039000      1.250521000
O        -4.189037000     -1.468867000      0.110874000
O        -1.662308000      2.133105000     -1.126952000
H        -3.682061000      0.713298000     -0.959019000
H        -1.963083000     -2.393799000      1.324161000
25
d4U 4
C         0.548087000      1.148764000      0.151902000
C         1.349109000      1.023292000      1.423893000
C         2.570621000      0.567678000      1.146022000
C         2.707561000      0.340041000     -0.335393000
O         1.391920000      0.595481000     -0.861222000
H         0.286239000      2.180924000     -0.096624000
H         0.951944000      1.306232000      2.391852000
H         3.383259000      0.395692000      1.841419000
H         3.415168000      1.059439000     -0.774418000
C         3.149730000     -1.065263000     -0.746161000
H         3.074564000     -1.151679000     -1.837988000
H         2.485197000     -1.812575000     -0.289561000
O         4.493888000     -1.220032000     -0.295526000
H         4.848163000     -2.057030000     -0.619456000
N        -0.738364000      0.434678000      0.174720000
N        -3.021855000      0.329102000     -0.314760000
C        -1.881723000      1.111352000     -0.280916000
C        -0.786978000     -0.903069000      0.512405000
C        -1.916537000     -1.642695000      0.462015000
C        -3.161580000     -1.032288000      0.019818000
H         0.160817000     -1.320476000      0.830912000
O        -4.250046000     -1.583293000     -0.073409000
O        -1.881803000      2.289125000     -0.606538000
H        -3.859073000      0.803252000     -0.635175000
H        -1.926151000     -2.687356000      0.741359000
25
d4U 5
C        -0.715249000     -1.192939000     -0.167743000
C        -1.467380000     -1.309160000      1.136145000
C        -2.698692000     -0.822383000      0.990037000
C        -2.888844000     -0.309422000     -0.414603000
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O       -1.604555000     -0.506590000     -1.039077000
H       -0.443366000     -2.169217000     -0.578768000
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H       -3.480383000     -0.800843000      1.742336000
H       -3.629822000     -0.916003000     -0.960857000
C       -3.328197000      1.154582000     -0.531683000
H       -4.388288000      1.230308000     -0.248371000
H       -3.234877000      1.463956000     -1.575816000
O       -2.528532000      2.062840000      0.220418000
H       -2.737364000      1.973791000      1.159624000
N        0.562021000     -0.455386000     -0.071598000
N        2.895085000     -0.434143000     -0.078758000
C        1.745882000     -1.197835000     -0.145420000
C        0.574948000      0.920003000      0.064750000
C        1.720847000      1.635559000      0.137571000
C        3.008025000      0.964332000      0.069126000
H       -0.405105000      1.385069000      0.086784000
O        4.113030000      1.488484000      0.126425000
O        1.766763000     -2.418424000     -0.248693000
H        3.763639000     -0.955066000     -0.127753000
H        1.706809000      2.712475000      0.235581000
25
d4U 6
C       -0.656009000     -1.321848000      0.065306000
C       -1.462971000     -1.154012000      1.328529000
C       -2.689409000     -0.745678000      1.012819000
C       -2.804405000     -0.526415000     -0.471935000
O       -1.462621000     -0.793725000     -0.966348000
H       -0.454029000     -2.386129000     -0.128236000
H       -1.071766000     -1.386862000      2.311590000
H       -3.506347000     -0.557224000      1.698844000
H       -3.475994000     -1.264047000     -0.939746000
C       -3.265314000      0.872673000     -0.893066000
H       -4.358102000      0.913375000     -0.812558000
H       -3.004392000      1.002294000     -1.955135000
O       -2.763725000      1.919426000     -0.091929000
H       -1.807059000      1.798954000      0.047011000
N        0.693393000     -0.709000000      0.044335000
N        2.172299000      1.090934000      0.250909000
C        0.865194000      0.651387000      0.321938000
C        1.773710000     -1.485690000     -0.338889000
C        3.041818000     -1.027020000     -0.415996000
C        3.327381000      0.363646000     -0.101253000
H        1.527750000     -2.514991000     -0.575024000
O        4.420625000      0.910203000     -0.123830000
O       -0.050839000      1.408043000      0.619607000
H        2.303326000      2.075542000      0.457481000
H        3.859288000     -1.668273000     -0.715653000
25
d4U 7
C        0.545233000      1.143072000      0.158308000
C        1.341053000      1.018231000      1.433833000
C        2.564550000      0.564608000      1.161306000
C        2.707369000      0.331853000     -0.318470000
O        1.393469000      0.585309000     -0.849972000
H        0.287527000      2.175566000     -0.093411000
H        0.938485000      1.297242000      2.400685000
H        3.371755000      0.389314000      1.862417000
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H	2.536085000	-1.826481000	-0.217831000
O	4.499501000	-1.330875000	-0.308712000
H	5.110322000	-0.931159000	-0.941002000
N	-0.741850000	0.432531000	0.175746000
N	-3.023348000	0.334154000	-0.323701000
C	-1.880928000	1.112226000	-0.286572000
C	-0.796239000	-0.905039000	0.515388000
C	-1.928103000	-1.640508000	0.461191000
C	-3.169255000	-1.026338000	0.013010000
H	0.148390000	-1.325836000	0.838666000
O	-4.259318000	-1.573210000	-0.083486000
O	-1.874855000	2.289392000	-0.614786000
H	-3.857613000	0.810444000	-0.648641000
H	-1.942241000	-2.684831000	0.741589000

25
d4U 8

C	-0.649375000	-1.301720000	-0.268345000
C	-1.363727000	-1.657694000	1.010290000
C	-2.576742000	-1.110858000	1.009252000
C	-2.773843000	-0.274469000	-0.223145000
O	-1.524781000	-0.421934000	-0.952910000
H	-0.480191000	-2.193779000	-0.887771000
H	-0.923457000	-2.293430000	1.768923000
H	-3.329617000	-1.211026000	1.782563000
H	-3.572212000	-0.665147000	-0.870455000
C	-3.039211000	1.209517000	0.037385000
H	-2.233707000	1.616801000	0.659559000
H	-3.989748000	1.317891000	0.570288000
O	-3.180968000	1.932479000	-1.179861000
H	-2.342879000	1.867290000	-1.658364000
N	0.701235000	-0.714254000	-0.130845000
N	2.215573000	0.860499000	0.712323000
C	0.920097000	0.371624000	0.733248000
C	1.712536000	-1.165815000	-0.961066000
C	2.963935000	-0.657132000	-0.969163000
C	3.303076000	0.441677000	-0.078237000
H	1.427295000	-1.980024000	-1.618364000
O	4.391234000	0.991251000	0.022255000
O	0.055741000	0.847268000	1.451734000
H	2.387581000	1.637934000	1.340655000
H	3.728986000	-1.043519000	-1.628436000

25
d4U 9

C	-2.926804000	0.140629000	0.412748000
O	-1.654318000	0.019987000	1.107598000
C	-0.740788000	0.988856000	0.631741000
C	-1.398558000	1.589226000	-0.586586000
C	-2.634426000	1.107562000	-0.699933000
C	-3.431948000	-1.240202000	-0.005894000
O	-2.696641000	-1.832720000	-1.063932000
H	-0.535634000	1.738793000	1.406212000
H	-0.900786000	2.321068000	-1.207801000
H	-3.359430000	1.357035000	-1.465852000
H	-3.654906000	0.557873000	1.126763000
H	-4.458510000	-1.137091000	-0.372330000

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C        1.614979000      1.172818000     -0.025007000
N        2.816153000      0.532727000     -0.259533000
C        3.110016000     -0.841225000     -0.130367000
C        1.969661000     -1.625341000      0.314954000
O        1.466916000      2.384154000     -0.137079000
H        2.106495000     -2.685647000      0.477455000
C        0.777179000     -1.023446000      0.539663000
H       -0.088136000     -1.559600000      0.906230000
H        3.581148000      1.135188000     -0.543117000
O        4.234633000     -1.257283000     -0.374609000
25
d4U 10
C        2.809276000      0.264982000     -0.067653000
O        1.677599000      0.136071000     -0.962119000
C        0.667100000      1.059523000     -0.630343000
C        1.201743000      1.836221000      0.547254000
C        2.418481000      1.388712000      0.853437000
C        3.101729000     -1.042626000      0.661062000
O        3.509044000     -2.009530000     -0.299773000
H        0.437448000      1.697475000     -1.490929000
H        0.641485000      2.636189000      1.012289000
H        3.061588000      1.754917000      1.645843000
H        3.681262000      0.512022000     -0.688671000
H        2.203473000     -1.366794000      1.205726000
H        3.899467000     -0.851325000      1.395431000
H        3.715663000     -2.838958000      0.148979000
N       -0.604435000      0.321447000     -0.318712000
C       -1.739420000      1.109743000     -0.138019000
N       -2.894752000      0.398296000      0.119877000
C       -3.053241000     -1.001983000      0.199667000
C       -1.817620000     -1.727525000     -0.040278000
O       -1.703736000      2.334386000     -0.197385000
H       -1.846000000     -2.808463000     -0.029313000
C       -0.669122000     -1.053714000     -0.291815000
H        0.269742000     -1.548420000     -0.504719000
H       -3.728320000      0.957895000      0.262543000
O       -4.152288000     -1.483769000      0.443628000
25
d4U 11
C        0.544206000      1.145363000      0.124083000
C        1.338783000      1.054385000      1.403291000
C        2.566783000      0.607225000      1.139692000
C        2.715868000      0.341828000     -0.335259000
O        1.396746000      0.572833000     -0.869051000
H        0.280709000      2.172193000     -0.145173000
H        0.936472000      1.359368000      2.362394000
H        3.374260000      0.485886000      1.853224000
H        3.417267000      1.058020000     -0.789271000
C        3.171089000     -1.072106000     -0.727752000
H        3.085219000     -1.174000000     -1.812775000
H        2.516141000     -1.822062000     -0.264173000
O        4.540042000     -1.293828000     -0.402189000
H        4.615392000     -1.570313000      0.519353000
N       -0.739932000      0.428970000      0.154416000
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C	-1.890747000	1.110386000	-0.275344000
C	-0.782958000	-0.911924000	0.480716000
C	-1.913276000	-1.650716000	0.442736000
C	-3.165645000	-1.035732000	0.027491000
H	0.170327000	-1.333348000	0.776052000
O	-4.255722000	-1.585255000	-0.050497000
O	-1.895291000	2.291765000	-0.587535000
H	-3.873274000	0.805449000	-0.600870000
H	-1.918315000	-2.698387000	0.710653000

25
d4U 12

C	2.814756000	0.251251000	-0.061543000
O	1.696467000	0.159999000	-0.972981000
C	0.685591000	1.077537000	-0.622179000
C	1.226838000	1.834716000	0.565506000
C	2.439705000	1.373609000	0.868252000
C	3.062712000	-1.078778000	0.661119000
O	3.256498000	-2.176458000	-0.217445000
H	0.453190000	1.728022000	-1.472036000
H	0.670162000	2.629403000	1.044034000
H	3.081948000	1.719674000	1.670268000
H	3.698798000	0.498379000	-0.670146000
H	2.191306000	-1.334421000	1.270407000
H	3.920509000	-0.948682000	1.339762000
H	4.045868000	-2.029273000	-0.755569000
N	-0.582837000	0.335312000	-0.316418000
C	-1.720330000	1.122248000	-0.146807000
N	-2.875819000	0.410430000	0.105936000
C	-3.030641000	-0.989973000	0.197981000
C	-1.790602000	-1.714255000	-0.022637000
O	-1.685012000	2.346971000	-0.211806000
H	-1.814520000	-2.795042000	0.002962000
C	-0.641773000	-1.040955000	-0.272721000
H	0.299151000	-1.538423000	-0.470877000
H	-3.711717000	0.968804000	0.239417000
O	-4.130657000	-1.471890000	0.436398000

25
d4U 13

C	0.620961000	1.155435000	0.047424000
C	1.298820000	1.342673000	1.381708000
C	2.530424000	0.836075000	1.333845000
C	2.799525000	0.259793000	-0.033068000
O	1.535457000	0.373010000	-0.717438000
H	0.405036000	2.100100000	-0.460239000
H	0.825321000	1.854757000	2.211271000
H	3.269424000	0.854278000	2.127241000
H	3.541745000	0.864162000	-0.577754000
C	3.298543000	-1.180110000	-0.029376000
H	2.483915000	-1.843303000	0.293173000
H	4.124526000	-1.262034000	0.695055000
O	3.743623000	-1.497706000	-1.341913000
H	3.905108000	-2.446952000	-1.406782000
N	-0.680481000	0.470660000	0.124404000
N	-2.932996000	0.292982000	-0.472691000
C	-1.780832000	1.056741000	-0.521294000
C	-0.777517000	-0.772201000	0.716367000
C	-1.918352000	-1.495535000	0.745899000
C	-3.122044000	-0.972479000	0.116690000

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H         0.141971000     -1.128835000      1.164677000
O        -4.215420000     -1.519714000      0.069319000
O        -1.737818000      2.149637000     -1.066352000
H        -3.739973000      0.702706000     -0.930204000
H        -1.966638000     -2.464547000      1.223478000
25
d4U 14
C         0.515329000      1.350204000      0.065251000
C         1.321360000      1.220368000      1.331914000
C         2.530537000      0.747673000      1.040937000
C         2.631571000      0.451650000     -0.428820000
O         1.341523000      0.830611000     -0.960917000
H         0.285751000      2.401908000     -0.156418000
H         0.934220000      1.504766000      2.302887000
H         3.343425000      0.556180000      1.730225000
H         3.397548000      1.072453000     -0.915005000
C         2.913722000     -1.014102000     -0.767708000
H         2.772486000     -1.155731000     -1.848015000
H         2.211352000     -1.654886000     -0.224564000
O         4.270601000     -1.261650000     -0.387400000
H         4.446400000     -2.208431000     -0.444958000
N        -0.815826000      0.698929000      0.060342000
N        -2.245405000     -1.133968000      0.341874000
C        -0.953738000     -0.644214000      0.446254000
C        -1.896287000      1.396021000     -0.449629000
C        -3.141976000      0.883730000     -0.558254000
C        -3.398150000     -0.485133000     -0.140131000
H        -1.672312000      2.410621000     -0.760624000
O        -4.470698000     -1.073021000     -0.178555000
O        -0.029420000     -1.331476000      0.850621000
H        -2.358807000     -2.100098000      0.628723000
H        -3.961705000      1.465587000     -0.956634000
25
d4U 15
C        -2.752521000      0.176072000      0.391448000
O        -1.512536000      0.146804000      1.141336000
C        -0.567007000      1.034422000      0.580504000
C        -1.217941000      1.571349000     -0.669998000
C        -2.454342000      1.084312000     -0.768630000
C        -3.157750000     -1.262483000      0.032209000
O        -4.463728000     -1.311546000     -0.531504000
H        -0.308547000      1.824717000      1.293289000
H        -0.713026000      2.265414000     -1.329244000
H        -3.176328000      1.312061000     -1.544832000
H        -3.535238000      0.595905000      1.038629000
H        -3.192124000     -1.855063000      0.950868000
H        -2.409624000     -1.706824000     -0.638093000
H        -4.416646000     -1.120306000     -1.476464000
N         0.712235000      0.304059000      0.312932000
C         1.820459000      1.105928000      0.039213000
N         2.988523000      0.406631000     -0.191897000
C         3.177621000     -0.992094000     -0.197629000
C         1.962445000     -1.730954000      0.102329000
O         1.750134000      2.329376000      0.001567000
H         2.013463000     -2.810435000      0.140312000
C         0.805655000     -1.068923000      0.343385000
H        -0.116969000     -1.574064000      0.595440000
H         3.803191000      0.975104000     -0.395966000
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O        4.281983000     -1.463025000     -0.436170000
25
d4U 16
C        0.627167000      1.153787000      0.025331000
C        1.304345000      1.363908000      1.356801000
C        2.541220000      0.869757000      1.315236000
C        2.808972000      0.268282000     -0.041882000
O        1.547325000      0.362974000     -0.726844000
H        0.409350000      2.090752000     -0.495745000
H        0.825077000      1.879691000      2.180775000
H        3.279327000      0.902509000      2.108929000
H        3.543667000      0.881147000     -0.594145000
C        3.319749000     -1.174388000     -0.002676000
H        2.563293000     -1.820188000      0.452058000
H        4.219257000     -1.202861000      0.633908000
O        3.577491000     -1.725662000     -1.283010000
H        4.258121000     -1.204504000     -1.729599000
N       -0.670082000      0.465695000      0.107732000
N       -2.932512000      0.301797000     -0.451601000
C       -1.779230000      1.061466000     -0.513357000
C       -0.759410000     -0.784523000      0.687173000
C       -1.902077000     -1.503704000      0.729419000
C       -3.115695000     -0.968815000      0.129945000
H        0.167880000     -1.151594000      1.109729000
O       -4.212549000     -1.509661000      0.098989000
O       -1.740771000      2.159758000     -1.048813000
H       -3.746363000      0.718544000     -0.890197000
H       -1.943647000     -2.479825000      1.192858000
25
d4U 17
C       -0.614508000     -1.329973000     -0.238735000
C       -1.322459000     -1.653050000      1.051608000
C       -2.533145000     -1.102210000      1.039092000
C       -2.730414000     -0.300998000     -0.219307000
O       -1.496037000     -0.489681000     -0.954133000
H       -0.426160000     -2.239833000     -0.826029000
H       -0.881540000     -2.270033000      1.825191000
H       -3.284639000     -1.177201000      1.816524000
H       -3.542791000     -0.702254000     -0.842621000
C       -3.012059000      1.177088000      0.026881000
H       -2.111056000      1.643718000      0.437477000
H       -3.824212000      1.258387000      0.766665000
O       -3.409982000      1.766306000     -1.210883000
H       -3.240254000      2.715058000     -1.178203000
N        0.731193000     -0.718278000     -0.114211000
N        2.216473000      0.916496000      0.661450000
C        0.926458000      0.413660000      0.691911000
C        1.755487000     -1.195277000     -0.912053000
C        3.000968000     -0.671624000     -0.934663000
C        3.317150000      0.474164000     -0.097236000
H        1.486417000     -2.043580000     -1.531992000
O        4.396835000      1.044005000     -0.013685000
O        0.048909000      0.918032000      1.375675000
H        2.371644000      1.727592000      1.250122000
H        3.776272000     -1.079349000     -1.568585000
25
d4U 18
C        0.520566000      1.366238000      0.089608000
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C         1.340351000      1.203810000      1.343642000
C         2.545296000      0.736395000      1.026998000
C         2.631557000      0.471670000     -0.450024000
O         1.340410000      0.884739000     -0.959419000
H         0.282927000      2.422921000     -0.096715000
H         0.967089000      1.469543000      2.325271000
H         3.364771000      0.547635000      1.710239000
H         3.400826000      1.095985000     -0.925766000
C         2.882912000     -0.994404000     -0.841095000
H         2.829195000     -1.076834000     -1.930890000
H         2.105616000     -1.626363000     -0.401724000
O         4.195816000     -1.402703000     -0.451310000
H         4.147466000     -1.842542000      0.405761000
N        -0.806903000      0.707710000      0.080086000
N        -2.226117000     -1.136014000      0.339473000
C        -0.938941000     -0.639027000      0.454415000
C        -1.888868000      1.402175000     -0.431765000
C        -3.130497000      0.883025000     -0.550940000
C        -3.380645000     -0.490379000     -0.143846000
H        -1.669019000      2.420115000     -0.734559000
O        -4.449188000     -1.084206000     -0.191342000
O        -0.012215000     -1.323674000      0.859758000
H        -2.335072000     -2.105203000      0.617770000
H        -3.951635000      1.462608000     -0.949756000
25
d4U 19
C         0.509906000      1.346608000      0.059343000
C         1.309057000      1.227962000      1.331828000
C         2.520062000      0.752672000      1.052745000
C         2.629277000      0.440716000     -0.412880000
O         1.341023000      0.810351000     -0.955768000
H         0.286462000      2.396718000     -0.176160000
H         0.915001000      1.516505000      2.298763000
H         3.325148000      0.561220000      1.751417000
H         3.389966000      1.069939000     -0.902610000
C         2.929857000     -1.033714000     -0.730290000
H         2.749645000     -1.211452000     -1.798505000
H         2.263139000     -1.676431000     -0.153358000
O         4.265677000     -1.370991000     -0.356222000
H         4.878535000     -1.041760000     -1.026032000
N        -0.821280000      0.699705000      0.054241000
N        -2.251173000     -1.132342000      0.342592000
C        -0.959981000     -0.641649000      0.448313000
C        -1.900253000      1.394798000     -0.461654000
C        -3.145450000      0.881572000     -0.569892000
C        -3.402408000     -0.485556000     -0.145360000
H        -1.675616000      2.407874000     -0.777209000
O        -4.475273000     -1.072682000     -0.183669000
O        -0.035908000     -1.323988000      0.859636000
H        -2.364933000     -2.097226000      0.633723000
H        -3.964722000      1.461090000     -0.972599000
25
d4U 20
C        -0.623690000     -1.332805000     -0.251801000
C        -1.345063000     -1.660808000      1.029872000
C        -2.551473000     -1.100552000      1.013830000
C        -2.727726000     -0.279731000     -0.235891000
O        -1.496419000     -0.478581000     -0.966537000
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H	-0.440789000	-2.238697000	-0.846708000
H	-0.913892000	-2.284907000	1.803173000
H	-3.307309000	-1.174501000	1.787089000
H	-3.542058000	-0.676067000	-0.865202000
C	-2.988553000	1.207068000	0.030478000
H	-2.110496000	1.641177000	0.511634000
H	-3.843159000	1.291236000	0.720905000
O	-3.214119000	1.957518000	-1.156227000
H	-4.033842000	1.660901000	-1.573083000
N	0.722494000	-0.731700000	-0.115427000
N	2.214485000	0.878705000	0.699120000
C	0.928351000	0.367345000	0.734440000
C	1.732736000	-1.168002000	-0.954324000
C	2.974513000	-0.636605000	-0.978446000
C	3.301450000	0.474970000	-0.099341000
H	1.455472000	-1.990392000	-1.604780000
O	4.380401000	1.045437000	-0.013209000
O	0.062460000	0.833280000	1.458078000
H	2.375872000	1.667890000	1.315370000
H	3.739486000	-1.012186000	-1.643990000

Cartesian coordinates of the 19 d4C structures optimised with B3LYP/6-31++G(d,p)

26
d4C 1

C	-2.915309000	-0.274474000	-0.327370000
O	-1.613935000	-0.593108000	-0.857595000
C	-0.784137000	-1.179951000	0.159963000
C	-1.582252000	-1.023906000	1.428953000
C	-2.774537000	-0.497139000	1.155585000
C	-3.312507000	1.134464000	-0.781895000
O	-2.354066000	2.120554000	-0.426453000
H	-0.561534000	-2.218474000	-0.098963000
H	-1.200217000	-1.330218000	2.395877000
H	-3.568347000	-0.284786000	1.863190000
H	-3.653255000	-0.979171000	-0.747718000
H	-4.255086000	1.419853000	-0.303251000
H	-3.474792000	1.122224000	-1.868420000
H	-1.552252000	1.928609000	-0.932594000
N	0.524155000	-0.519494000	0.191113000
C	1.667846000	-1.228899000	-0.336474000
N	2.855580000	-0.550565000	-0.373647000
C	2.939908000	0.696771000	0.049825000
C	1.821893000	1.429064000	0.581549000
N	4.154386000	1.300730000	-0.040291000
O	1.526441000	-2.386944000	-0.708835000
H	1.907559000	2.451205000	0.929160000
H	4.934069000	0.754830000	-0.375123000
H	4.316713000	2.224791000	0.323027000
C	0.635111000	0.768317000	0.623566000
H	-0.275318000	1.226937000	0.995426000

26
d4C 2

C	2.742004000	0.297957000	-0.343567000
O	1.432948000	0.477232000	-0.911681000
C	0.566170000	1.124851000	0.029002000

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C         1.341127000      1.109842000      1.323451000
C         2.570186000      0.638576000      1.113013000
C         3.224449000     -1.123001000     -0.637391000
O         4.567094000     -1.211277000     -0.162354000
H         0.310836000      2.132055000     -0.311644000
H         0.919385000      1.469527000      2.254819000
H         3.367775000      0.528221000      1.837873000
H         3.443514000      0.997204000     -0.824436000
H         3.165402000     -1.296814000     -1.719870000
H         2.573291000     -1.849406000     -0.130002000
H         4.944625000     -2.060259000     -0.422086000
N        -0.722839000      0.421300000      0.083762000
C        -1.923050000      1.141672000     -0.267968000
N        -3.091835000      0.430154000     -0.280620000
C        -3.110078000     -0.852664000      0.029435000
C        -1.935322000     -1.592895000      0.401941000
N        -4.312160000     -1.487272000     -0.030511000
O        -1.843969000      2.337580000     -0.522853000
H        -1.966044000     -2.645893000      0.652899000
H        -5.130776000     -0.930817000     -0.226734000
H        -4.427106000     -2.432189000      0.295760000
C        -0.766376000     -0.899442000      0.403456000
H         0.183698000     -1.358568000      0.651872000
26
d4C 3
C         0.767248000      1.100615000     -0.458980000
C         1.450942000      1.485864000      0.830045000
C         2.674572000      0.958701000      0.860670000
C         2.930307000      0.166493000     -0.396411000
O         1.689444000      0.253207000     -1.126227000
H         0.527347000      1.974250000     -1.072633000
H         0.971811000      2.123641000      1.562077000
H         3.414922000      1.080290000      1.644719000
H         3.719149000      0.635941000     -1.006814000
C         3.335722000     -1.296014000     -0.185334000
H         4.347612000     -1.318053000      0.248289000
H         3.374263000     -1.798272000     -1.155517000
O         2.419273000     -2.045467000      0.603068000
H         2.349422000     -1.641587000      1.479207000
N        -0.523100000      0.396786000     -0.257322000
N        -2.879738000      0.610537000      0.082907000
C        -1.669371000      1.228678000     -0.041204000
C        -0.614447000     -0.958236000     -0.247178000
C        -1.822398000     -1.568014000     -0.081374000
C        -2.961636000     -0.710000000      0.064672000
H         0.314693000     -1.501019000     -0.373735000
O        -1.493231000      2.444788000      0.026846000
H        -1.905050000     -2.647770000     -0.083442000
N        -4.207457000     -1.251504000      0.171642000
H        -4.974911000     -0.626789000      0.369054000
H        -4.336710000     -2.240103000      0.309267000
26
d4C 4
C         0.675144000      1.020625000     -0.476965000
C         1.215533000      1.713133000      0.749462000
C         2.454850000      1.289946000      0.995173000
C         2.873837000      0.280190000     -0.037052000
O         1.684212000      0.090710000     -0.848070000
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H         0.471161000      1.720155000     -1.293428000
H         0.637641000      2.454328000      1.286402000
H         3.105735000      1.619344000      1.797470000
H         3.663206000      0.671890000     -0.695943000
C         3.328544000     -1.073910000      0.503028000
H         2.545729000     -1.490226000      1.155333000
H         4.235690000     -0.944131000      1.102103000
O         3.664362000     -1.975811000     -0.542044000
H         2.922027000     -2.004735000     -1.162285000
N        -0.608742000      0.313247000     -0.237204000
N        -2.989892000      0.497629000     -0.094305000
C        -1.790917000      1.125822000     -0.270622000
C        -0.672719000     -1.013667000      0.033828000
C        -1.870084000     -1.628894000      0.244018000
C        -3.038667000     -0.800986000      0.150539000
H         0.273182000     -1.539267000      0.052138000
O        -1.651554000      2.334112000     -0.447866000
H        -1.924987000     -2.691396000      0.445338000
N        -4.273066000     -1.356619000      0.295343000
H        -5.069230000     -0.736713000      0.308429000
H        -4.387532000     -2.304694000      0.613005000
26
d4C 5
C        -0.687883000     -1.324211000      0.085166000
C        -1.494168000     -1.115730000      1.342101000
C        -2.715084000     -0.699207000      1.016696000
C        -2.822386000     -0.499778000     -0.471313000
O        -1.491727000     -0.819368000     -0.961685000
H        -0.502823000     -2.397667000     -0.079817000
H        -1.105068000     -1.325023000      2.331207000
H        -3.527960000     -0.480295000      1.698455000
H        -3.517919000     -1.220654000     -0.930919000
C        -3.238984000      0.909525000     -0.909954000
H        -4.332460000      0.976968000     -0.850183000
H        -2.957208000      1.019870000     -1.969631000
O        -2.726098000      1.950373000     -0.112097000
H        -1.773926000      1.804830000      0.053780000
N         0.665024000     -0.726798000      0.047611000
N         2.158997000      1.131680000      0.286229000
C         0.877883000      0.664564000      0.335369000
C         1.708215000     -1.507701000     -0.353682000
C         2.978321000     -1.030837000     -0.432425000
C         3.158929000      0.346754000     -0.072225000
H         1.464716000     -2.535400000     -0.602621000
O        -0.084152000      1.371376000      0.624752000
H         3.797596000     -1.665677000     -0.745681000
N         4.404417000      0.890785000     -0.076773000
H         4.487440000      1.880947000      0.100490000
H         5.195304000      0.393104000     -0.450705000
26
d4C 6
C  0.00000000    0.00000000    0.00000000
O  0.00000000    0.00000000    1.44547837
C  1.34270433    0.00000000    1.95007646
C  2.19875033   -0.22648840    0.72893593
C  1.44185970   -0.22526073   -0.36852765
C  -0.98451392  -1.05955957   -0.49369469
O  -2.30266968  -0.80661336   -0.03515342
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H  1.56059879    0.94192837    2.46107764
H  3.27541591    -0.33553360   0.78919282
H  1.78395019    -0.33461759   -1.39183362
H  -0.35308599   0.98584895    -0.34034417
H  -0.63792318   -2.05581543   -0.17776556
H  -1.02676840   -1.04399230   -1.58783950
H  -2.26611894   -0.71338007   0.92801251
N  1.48905455    -1.02243410   2.99348528
C  1.85453972    -0.60360302   4.32667844
N  1.89662527    -1.57311605   5.29079814
C  1.63541264    -2.83365755   4.99981859
C  1.28687272    -3.28464029   3.67947007
N  1.72534996    -3.73582420   6.01467307
O  2.11133894    0.57739554    4.52677369
H  1.07973308    -4.32358341   3.45514478
H  1.87817923    -3.37825688   6.94625980
H  1.39672734    -4.68097397   5.90488831
C  1.22208554    -2.32765321   2.71720106
H  0.95327881    -2.55098226   1.69093311
26
d4C 7
C       -0.732198000     -1.199533000     -0.137229000
C       -1.485272000     -1.288028000      1.166696000
C       -2.701429000     -0.765059000      1.026406000
C       -2.897007000     -0.296128000     -0.392859000
O       -1.617602000     -0.504172000     -1.017337000
H       -0.466972000     -2.177923000     -0.545912000
H       -1.050886000     -1.731566000      2.054618000
H       -3.469220000     -0.684712000      1.787418000
H       -3.638310000     -0.926214000     -0.912690000
C       -3.362116000      1.145711000     -0.567166000
H       -4.417976000      1.206414000     -0.262919000
H       -3.289643000      1.403833000     -1.631738000
O       -2.558026000      2.017991000      0.228233000
H       -2.780543000      2.932231000      0.013624000
N        0.548732000     -0.477392000     -0.039602000
N        2.939037000     -0.524364000     -0.141624000
C        1.767253000     -1.229221000     -0.172885000
C        0.561836000      0.867063000      0.168959000
C        1.737003000      1.551686000      0.227552000
C        2.935020000      0.783211000      0.045810000
H       -0.407887000      1.345314000      0.263303000
O        1.700133000     -2.449123000     -0.295752000
H        1.753217000      2.623818000      0.380245000
N        4.145035000      1.412718000      0.034827000
H        4.969652000      0.830770000      0.018441000
H        4.234364000      2.365506000      0.347546000
26
d4C 8
C        0.755245000      0.980368000     -0.606529000
C        1.405047000      1.556505000      0.628056000
C        2.643704000      1.080432000      0.736609000
C        2.946962000      0.140841000     -0.397957000
O        1.675455000      0.012427000     -1.088578000
H        0.566818000      1.747995000     -1.367349000
H        0.896304000      2.271748000      1.259416000
H        3.364990000      1.318765000      1.509783000
H        3.669112000      0.583386000     -1.103632000
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C	3.471683000	-1.242044000	-0.013266000
H	4.492031000	-1.135715000	0.369287000
H	3.515208000	-1.863744000	-0.919609000
O	2.730760000	-1.879347000	1.015701000
H	1.804512000	-1.930491000	0.745419000
N	-0.557561000	0.327607000	-0.348741000
N	-2.851211000	0.632074000	0.260848000
C	-1.634161000	1.201160000	0.018751000
C	-0.762903000	-0.999439000	-0.538981000
C	-1.986269000	-1.558978000	-0.317760000
C	-3.028047000	-0.669309000	0.107926000
H	0.091317000	-1.564202000	-0.890823000
O	-1.392996000	2.403318000	0.103761000
H	-2.154865000	-2.616083000	-0.480669000
N	-4.278110000	-1.155911000	0.344435000
H	-4.961561000	-0.520398000	0.728777000
H	-4.449003000	-2.146037000	0.405450000

26
d4C 9

C	-0.583523000	0.999080000	0.568192000
C	-1.240143000	1.541901000	-0.676714000
C	-2.476361000	1.054781000	-0.776608000
C	-2.769045000	0.146394000	0.384865000
O	-1.523643000	0.086518000	1.115592000
H	-0.341694000	1.785403000	1.290848000
H	-0.731621000	2.236307000	-1.332391000
H	-3.205214000	1.261197000	-1.551072000
H	-3.538819000	0.574002000	1.043693000
C	-3.204229000	-1.272609000	0.014875000
H	-3.215431000	-1.887336000	0.925667000
H	-2.487891000	-1.705159000	-0.698187000
O	-4.505968000	-1.165281000	-0.557842000
H	-4.834295000	-2.045637000	-0.777313000
N	0.701932000	0.296446000	0.300389000
N	3.034619000	0.521804000	-0.179047000
C	1.834291000	1.135326000	0.039663000
C	0.810724000	-1.053973000	0.312097000
C	2.008730000	-1.661754000	0.078151000
C	3.127057000	-0.797192000	-0.163591000
H	-0.098694000	-1.597118000	0.534562000
O	1.654964000	2.351486000	0.020470000
H	2.102864000	-2.740213000	0.103284000
N	4.365137000	-1.331968000	-0.362684000
H	5.106565000	-0.701641000	-0.630405000
H	4.484578000	-2.317289000	-0.530635000

26
d4C 10

C	2.739954000	0.288500000	-0.327280000
O	1.432564000	0.468448000	-0.898741000
C	0.563961000	1.120692000	0.038431000
C	1.335940000	1.105735000	1.334781000
C	2.565659000	0.634757000	1.127396000
C	3.228729000	-1.138448000	-0.612798000
O	4.572930000	-1.327398000	-0.177756000
H	0.312837000	2.128100000	-0.305003000
H	0.910988000	1.461943000	2.266005000
H	3.358781000	0.519901000	1.856673000
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H         3.111346000     -1.350315000     -1.683382000
H         2.622687000     -1.859118000     -0.056101000
H         5.175005000     -0.919445000     -0.813405000
N        -0.725966000      0.421115000      0.090176000
C        -1.921459000      1.142343000     -0.275872000
N        -3.091186000      0.432722000     -0.297210000
C        -3.115894000     -0.846706000      0.025539000
C        -1.946085000     -1.587820000      0.411383000
N        -4.327251000     -1.468326000      0.003966000
O        -1.836697000      2.336002000     -0.539417000
H        -1.983502000     -2.636384000      0.679244000
H        -5.110015000     -0.950707000     -0.368130000
H        -4.400241000     -2.469646000      0.078111000
C        -0.775079000     -0.898312000      0.416714000
H         0.171335000     -1.358935000      0.675862000
26
d4C 11
C        -0.578936000      1.003373000      0.550775000
C        -1.230350000      1.536710000     -0.701157000
C        -2.467765000      1.052508000     -0.801238000
C        -2.766582000      0.153895000      0.366060000
O        -1.523444000      0.095323000      1.100586000
H        -0.339015000      1.794934000      1.268111000
H        -0.716540000      2.220314000     -1.364185000
H        -3.189775000      1.249951000     -1.584617000
H        -3.529770000      0.599475000      1.025680000
C        -3.214211000     -1.269745000      0.003555000
H        -3.176493000     -1.898333000      0.903657000
H        -2.535857000     -1.694051000     -0.742285000
O        -4.509400000     -1.274910000     -0.589160000
H        -5.176129000     -1.141205000      0.097099000
N         0.705277000      0.297845000      0.293592000
N         3.045094000      0.517682000     -0.151743000
C         1.844933000      1.134303000      0.056812000
C         0.805564000     -1.053724000      0.281525000
C         2.003028000     -1.664101000      0.053772000
C         3.129934000     -0.802072000     -0.156489000
H        -0.109466000     -1.596160000      0.481461000
O         1.670762000      2.351441000      0.047995000
H         2.090111000     -2.743406000      0.059416000
N         4.367117000     -1.340772000     -0.346562000
H         5.118084000     -0.711315000     -0.588251000
H         4.485394000     -2.325205000     -0.520143000
26
d4C 12
C         0.700112000      1.057589000     -0.614783000
C         1.243312000      1.810613000      0.574247000
C         2.456753000      1.350223000      0.875532000
C         2.833019000      0.230140000     -0.057627000
O         1.710633000      0.127499000     -0.958915000
H         0.482781000      1.713842000     -1.464106000
H         0.682306000      2.603091000      1.050718000
H         3.100409000      1.696395000      1.676527000
H         3.713384000      0.484443000     -0.670472000
C         3.101040000     -1.095724000      0.663683000
H         2.231960000     -1.367816000      1.269107000
H         3.954638000     -0.951596000      1.345259000
O         3.320769000     -2.191339000     -0.213789000
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N       -0.572250000      0.335442000     -0.319472000
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C       -1.734882000      1.152440000     -0.146116000
C       -0.643872000     -1.018882000     -0.280487000
C       -1.830247000     -1.645316000     -0.036108000
C       -2.972738000     -0.801417000      0.158585000
H        0.282126000     -1.548000000     -0.469799000
O       -1.594201000      2.372614000     -0.222451000
H       -1.895861000     -2.725975000     -0.016640000
N       -4.195172000     -1.359365000      0.386039000
H       -4.957597000     -0.737880000      0.611686000
H       -4.288656000     -2.338765000      0.598704000
26
d4C 13
C       -0.680587000     -1.300562000     -0.277033000
C       -1.396530000     -1.650060000      1.002074000
C       -2.606519000     -1.096844000      1.002117000
C       -2.792897000     -0.246787000     -0.222817000
O       -1.553154000     -0.415458000     -0.961886000
H       -0.528318000     -2.196886000     -0.897089000
H       -0.958498000     -2.285192000      1.762443000
H       -3.357855000     -1.189744000      1.777848000
H       -3.603982000     -0.610836000     -0.870214000
C       -3.020650000      1.240292000      0.057659000
H       -2.203380000      1.617186000      0.682523000
H       -3.969223000      1.366804000      0.590381000
O       -3.141957000      1.981183000     -1.153194000
H       -2.296519000      1.911951000     -1.617891000
N        0.672735000     -0.725762000     -0.146423000
N        2.205242000      0.876676000      0.775919000
C        0.930316000      0.378085000      0.748390000
C        1.653948000     -1.179834000     -0.977089000
C        2.910169000     -0.662446000     -0.958562000
C        3.143394000      0.398972000     -0.018755000
H        1.373559000     -1.982491000     -1.651874000
O        0.014648000      0.809284000      1.435741000
H        3.682991000     -1.041078000     -1.615674000
N        4.387704000      0.940425000      0.090308000
H        4.494683000      1.749913000      0.683828000
H        5.106606000      0.736030000     -0.584106000
26
d4C 14
C        0.676748000      1.033540000     -0.612720000
C        1.214252000      1.804772000      0.566734000
C        2.436471000      1.365401000      0.862325000
C        2.830936000      0.250311000     -0.068914000
O        1.686439000      0.097500000     -0.939132000
H        0.462162000      1.679613000     -1.471140000
H        0.647700000      2.598051000      1.035020000
H        3.083745000      1.734517000      1.650180000
H        3.688818000      0.515980000     -0.703129000
C        3.165946000     -1.050946000      0.652078000
H        2.279263000     -1.404208000      1.197542000
H        3.960456000     -0.839529000      1.384519000
O        3.600726000     -2.004383000     -0.312216000
H        3.834227000     -2.826701000      0.136165000
N       -0.599236000      0.316822000     -0.314441000
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N	-2.945420000	0.506097000	0.107574000
C	-1.760676000	1.136752000	-0.143901000
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C	-1.864513000	-1.661094000	-0.037843000
C	-3.004224000	-0.814298000	0.160092000
H	0.248791000	-1.564709000	-0.472834000
O	-1.619102000	2.356158000	-0.223461000
H	-1.934319000	-2.741630000	-0.024242000
N	-4.228589000	-1.368958000	0.387450000
H	-4.988236000	-0.744970000	0.615647000
H	-4.324726000	-2.347816000	0.601319000

26
d4C 15

C	-0.590516000	1.001737000	0.614914000
C	-1.251020000	1.577305000	-0.613065000
C	-2.484691000	1.085756000	-0.724674000
C	-2.771944000	0.130890000	0.401205000
O	-1.532913000	0.085749000	1.147988000
H	-0.342122000	1.772165000	1.352912000
H	-0.748555000	2.297192000	-1.245118000
H	-3.211110000	1.339178000	-1.489080000
H	-3.561040000	0.514461000	1.063637000
C	-3.156387000	-1.297387000	-0.016646000
H	-3.196327000	-1.926354000	0.877193000
H	-2.392892000	-1.705111000	-0.693374000
O	-4.454542000	-1.348053000	-0.599921000
H	-4.405904000	-1.053668000	-1.518153000
N	0.690062000	0.298337000	0.321070000
N	3.005330000	0.527121000	-0.234383000
C	1.808372000	1.137353000	0.006043000
C	0.814094000	-1.049829000	0.387009000
C	2.010742000	-1.654546000	0.139364000
C	3.111310000	-0.790148000	-0.174521000
H	-0.081564000	-1.592783000	0.660058000
O	1.618562000	2.351778000	-0.036485000
H	2.116711000	-2.730263000	0.203701000
N	4.343939000	-1.320996000	-0.404616000
H	5.079691000	-0.695093000	-0.696155000
H	4.479179000	-2.313544000	-0.500548000

26
d4C 16

C	0.544325000	1.358568000	0.063993000
C	1.346510000	1.212874000	1.331012000
C	2.553275000	0.734099000	1.040719000
C	2.651182000	0.434119000	-0.428617000
O	1.374653000	0.848437000	-0.965561000
H	0.327915000	2.416285000	-0.148321000
H	0.957290000	1.488066000	2.303779000
H	3.360777000	0.528303000	1.732197000
H	3.435498000	1.030925000	-0.916135000
C	2.889633000	-1.041489000	-0.760005000
H	2.740138000	-1.185129000	-1.839071000
H	2.169981000	-1.655486000	-0.210240000
O	4.243017000	-1.330504000	-0.388094000
H	4.359593000	-2.287371000	-0.356072000
N	-0.788178000	0.716103000	0.047184000
N	-2.226083000	-1.178191000	0.378902000
C	-0.960001000	-0.659778000	0.447671000

C	-1.838858000	1.417501000	-0.463526000
C	-3.086143000	0.885122000	-0.555438000
C	-3.232050000	-0.465165000	-0.089243000
H	-1.622202000	2.430110000	-0.788817000
O	0.013356000	-1.293797000	0.832499000
H	-3.914026000	1.459241000	-0.952175000
N	-4.461120000	-1.052840000	-0.099607000
H	-4.509554000	-2.034325000	0.131266000
H	-5.233184000	-0.634319000	-0.591900000

26
d4C 17

C	0.552203000	1.373578000	0.093981000
C	1.370196000	1.186259000	1.345285000
C	2.571780000	0.713847000	1.024157000
C	2.652060000	0.455654000	-0.454594000
O	1.374213000	0.907565000	-0.962885000
H	0.328593000	2.437293000	-0.076126000
H	0.996810000	1.437052000	2.330740000
H	3.387602000	0.504887000	1.705786000
H	3.438524000	1.059747000	-0.928792000
C	2.858173000	-1.017237000	-0.847966000
H	2.823861000	-1.094158000	-1.939180000
H	2.049308000	-1.618643000	-0.424133000
O	4.148526000	-1.475998000	-0.432977000
H	4.059285000	-1.924056000	0.416519000
N	-0.777220000	0.725438000	0.070436000
N	-2.207165000	-1.178543000	0.376879000
C	-0.944946000	-0.654539000	0.457239000
C	-1.828434000	1.426177000	-0.441317000
C	-3.071974000	0.888016000	-0.546111000
C	-3.213981000	-0.467042000	-0.092529000
H	-1.614707000	2.442535000	-0.756575000
O	0.029763000	-1.287273000	0.842944000
H	-3.900296000	1.461148000	-0.943350000
N	-4.439148000	-1.061339000	-0.116830000
H	-4.484121000	-2.044881000	0.105991000
H	-5.210608000	-0.642449000	-0.609804000

26
d4C 18

C	0.537036000	1.349696000	0.056675000
C	1.329551000	1.218089000	1.331701000
C	2.539395000	0.737932000	1.056846000
C	2.648922000	0.420383000	-0.407748000
O	1.373089000	0.816735000	-0.958298000
H	0.329994000	2.405725000	-0.173497000
H	0.930984000	1.498964000	2.299000000
H	3.337974000	0.534426000	1.759580000
H	3.425906000	1.029910000	-0.898042000
C	2.918721000	-1.062160000	-0.716491000
H	2.725209000	-1.243266000	-1.782059000
H	2.245430000	-1.687534000	-0.128949000
O	4.254191000	-1.421552000	-0.355657000
H	4.865402000	-1.081594000	-1.021653000
N	-0.796280000	0.714545000	0.038914000
N	-2.238078000	-1.174982000	0.381894000
C	-0.971321000	-0.658189000	0.451649000
C	-1.843811000	1.414419000	-0.480503000
C	-3.091404000	0.883019000	-0.571673000

C	-3.240743000	-0.463960000	-0.095533000
H	-1.624494000	2.424256000	-0.812736000
O	0.000338000	-1.287503000	0.845827000
H	-3.917531000	1.455286000	-0.974693000
N	-4.470942000	-1.049432000	-0.105949000
H	-4.521217000	-2.029411000	0.131166000
H	-5.239568000	-0.634498000	-0.606646000

26
d4C 19

C	-0.653548000	-1.332167000	-0.264262000
C	-1.374799000	-1.654310000	1.018442000
C	-2.576448000	-1.084224000	1.007238000
C	-2.742912000	-0.248180000	-0.233904000
O	-1.525344000	-0.472788000	-0.978285000
H	-0.487741000	-2.241642000	-0.860988000
H	-0.945623000	-2.279735000	1.791665000
H	-3.328721000	-1.149418000	1.784713000
H	-3.573865000	-0.614872000	-0.860251000
C	-2.959797000	1.242532000	0.050024000
H	-2.055254000	1.650618000	0.503970000
H	-3.790014000	1.344089000	0.767418000
O	-3.209243000	2.004959000	-1.126839000
H	-4.042817000	1.717074000	-1.521689000
N	0.695076000	-0.742611000	-0.135049000
N	2.211583000	0.880103000	0.777350000
C	0.945080000	0.360058000	0.762470000
C	1.669087000	-1.165878000	-0.989548000
C	2.915145000	-0.623926000	-0.987508000
C	3.144061000	0.430642000	-0.039657000
H	1.391586000	-1.964768000	-1.669889000
O	0.032488000	0.770091000	1.467305000
H	3.683002000	-0.978466000	-1.663605000
N	4.381432000	0.993094000	0.057054000
H	4.473970000	1.808772000	0.644842000
H	5.080427000	0.828873000	-0.648894000