



Supporting Information is available under the Creative Commons Attribution-Noncommercial NoDerivs 3.0 license CC BY-NC-ND 3.0.

Supporting Information

Please note:

- 1) The publisher is not responsible for the content of the section Supporting Information.
- 2) Any queries should be directed to the corresponding Authors mentioned below.

Research paper

A Theoretical Study of Polyethylene Glycol Polynitrates as Potential Highly Energetic Plasticizers for Propellants

Guixiang Wang*, **Yimin Xu**, **Wenjing Zhang**, **Xuedong Gong****

Computation Institute for Molecules and Materials, Department of Chemistry, Nanjing University of Science and Technology, Nanjing 210094, China
*E-mails: *wanggx1028@163.com; **gongxd325@mail.njust.edu.cn*

Content

Table S1. Thermodynamic properties of the title compounds at different temperatures

Table S2. The geometric parameters of reactant

Table S3. The geometric parameters of TS

Table S4. The geometric parameters of products

Table S1. Thermodynamic properties of the title compounds at different temperatures

Chemical name	Parameter	Temperature [K]							
		200	298.15	300	400	500	600	700	800
EGDN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	111.26	143.95	144.56	175.61	201.51	222.24	238.77	252.08
	S_m^o [J·(mol·K) ⁻¹]	372.93	423.42	424.31	470.25	512.32	550.97	586.51	619.29
	H_m^o [a.u.]	-639.0854	-639.0807	-639.0806	-639.0745	-639.0673	-639.0592	-639.0504	-639.0410
DEGDN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	151.60	198.68	199.58	246.60	287.07	320.12	346.93	368.84
	S_m^o [J·(mol·K) ⁻¹]	448.34	517.54	518.77	582.74	642.25	697.61	749.04	796.85
	H_m^o [a.u.]	-792.8570	-792.8505	-792.8503	-792.8418	-792.8316	-792.8200	-792.8073	-792.7937
DEGTN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	231.88	301.61	302.88	366.11	417.46	457.73	489.28	514.29
	S_m^o [J·(mol·K) ⁻¹]	583.93	689.61	691.48	787.53	874.96	954.78	1027.81	1094.84
	H_m^o [a.u.]	-1352.1997	-1352.1897	-1352.1895	-1352.1767	-1352.1617	-1352.1450	-1352.1270	-1352.1078
TriEGDN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	194.35	254.32	255.50	317.77	372.49	417.74	454.77	485.27
	S_m^o [J·(mol·K) ⁻¹]	524.84	613.39	614.96	697.10	774.06	846.11	913.37	976.15
	H_m^o [a.u.]	-946.6272	-946.6188	-946.6186	-946.6077	-946.5945	-946.5794	-946.5628	-946.5449
TriEGHN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	353.58	460.04	461.95	556.98	633.51	693.21	739.73	776.41
	S_m^o [J·(mol·K) ⁻¹]	788.39	949.63	952.48	1098.81	1231.66	1352.66	1463.16	1564.43
	H_m^o [a.u.]	-2065.3132	-2065.2980	-2065.2977	-2065.2782	-2065.2555	-2065.2302	-2065.2028	-2065.1739

Table S1. continuation

Chemical name	Parameter	Temperature [K]							
		200	298.15	300	400	500	600	700	800
TetraEGDN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	235.89	309.76	311.22	389.12	458.18	515.59	562.76	601.74
	S_m^o [J·(mol·K) ⁻¹]	594.51	702.14	704.06	804.37	898.83	987.61	1070.75	1148.52
	H_m^o [a.u.]	-1100.3971	-1100.3870	-1100.3867	-1100.3734	-1100.3572	-1100.3386	-1100.3181	-1100.2959
TetraEGON	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	471.61	615.47	618.05	745.95	848.41	927.94	989.67	1038.15
	S_m^o [J·(mol·K) ⁻¹]	938.10	1153.54	1157.35	1353.25	1531.18	1693.20	1841.07	1976.51
	H_m^o [a.u.]	-2778.4290	-2778.4086	-2778.4082	-2778.3821	-2778.3517	-2778.3178	-2778.2812	-2778.2426
PEGDN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	281.13	366.00	367.71	460.13	543.22	612.81	670.28	717.94
	S_m^o [J·(mol·K) ⁻¹]	677.14	804.71	806.98	925.51	1037.35	1142.74	1241.66	1334.37
	H_m^o [a.u.]	-1254.1656	-1254.1535	-1254.1533	-1254.1375	-1254.1184	-1254.0963	-1254.0718	-1254.0454
PEGDeN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	597.22	776.57	779.78	938.41	1065.42	1164.04	1240.55	1300.60
	S_m^o [J·(mol·K) ⁻¹]	1193.61	1465.96	1470.77	1717.55	1941.17	2144.52	2329.95	2499.68
	H_m^o [a.u.]	-3491.5436	-3491.5179	-3491.5173	-3491.4845	-3491.4462	-3491.4037	-3491.3579	-3491.3094
HEGDN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	323.01	421.77	423.77	531.65	628.99	710.73	778.37	834.57
	S_m^o [J·(mol·K) ⁻¹]	750.02	896.81	899.43	1036.20	1165.57	1287.71	1402.51	1510.23
	H_m^o [a.u.]	-1407.9345	-1407.9206	-1407.9203	-1407.9021	-1407.8800	-1407.8544	-1407.8260	-1407.7953
HEGDoN	$C_{p,m}^o$ [J·(mol·K) ⁻¹]	716.88	933.98	937.85	1128.93	1281.45	1399.62	1491.14	1562.88
	S_m^o [J·(mol·K) ⁻¹]	1393.94	1721.23	1727.02	2023.89	2292.89	2537.43	2760.35	2964.33
	H_m^o [a.u.]	-4204.6547	-4204.6238	-4204.6231	-4204.5836	-4204.5376	-4204.4865	-4204.4313	-4204.3731

Table S2. The geometric parameters of reactant

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
H(18)-C(1)	1.091	H(18)-C(1)-H(17)	107.677	N(14)-O(13)-C(1)-C(2)	-95.903
H(17)-C(1)	1.093	H(18)-C(1)-O(13)	109.500	N(14)-O(13)-C(1)-H(17)	143.722
O(13)-C(1)	1.429	H(18)-C(1)-C(2)	110.400	N(14)-O(13)-C(1)-H(18)	25.874
C(2)-C(1)	1.526	H(17)-C(1)-O(13)	109.500	O(3)-C(2)-C(1)-O(13)	65.096
O(40)-N(38)	1.199	H(17)-C(1)-C(2)	109.272	O(3)-C(2)-C(1)-H(17)	-174.393
O(36)-N(35)	1.211	O(13)-C(1)-C(2)	110.441	O(3)-C(2)-C(1)-H(18)	-56.148
O(33)-N(32)	1.206	N(32)-O(33)-N(29)	102.922	O(28)-C(2)-C(1)-O(13)	-179.015
O(33)-N(29)	3.408	O(40)-N(38)-O(39)	130.866	O(28)-C(2)-C(1)-H(17)	-58.504
O(30)-N(29)	1.208	O(40)-N(38)-O(28)	111.815	O(28)-C(2)-C(1)-H(18)	59.742
O(15)-N(14)	1.201	O(39)-N(38)-O(28)	117.297	H(19)-C(2)-C(1)-O(13)	-58.704
O(39)-N(38)	1.211	O(36)-N(35)-O(37)	130.876	H(19)-C(2)-C(1)-H(17)	61.807
O(37)-N(35)	1.197	O(36)-N(35)-O(27)	117.585	H(19)-C(2)-C(1)-H(18)	-179.948
O(34)-N(32)	1.196	O(37)-N(35)-O(27)	111.532	N(29)-O(33)-N(32)-O(26)	-59.984
O(31)-N(29)	1.197	O(33)-N(32)-O(34)	131.466	N(29)-O(33)-N(32)-O(34)	119.554
O(16)-N(14)	1.209	O(33)-N(32)-O(26)	117.801	N(32)-O(33)-N(29)-O(25)	65.628
N(38)-O(28)	1.447	O(34)-N(32)-O(26)	110.732	N(32)-O(33)-N(29)-O(31)	-178.047
O(27)-N(35)	1.455	O(33)-N(29)-O(30)	62.834	N(32)-O(33)-N(29)-O(30)	-51.996
O(26)-N(32)	1.471	O(33)-N(29)-O(31)	112.335	O(39)-N(38)-O(28)-C(2)	-10.832
O(25)-N(29)	1.465	O(33)-N(29)-O(25)	97.296	O(40)-N(38)-O(28)-C(2)	170.695
O(13)-N(14)	1.448	O(30)-N(29)-O(31)	131.133	C(4)-O(27)-N(35)-O(37)	-170.893
H(24)-C(8)	1.093	O(30)-N(29)-O(25)	117.850	C(4)-O(27)-N(35)-O(36)	9.979
H(23)-C(8)	1.093	O(31)-N(29)-O(25)	111.015	C(5)-O(26)-N(32)-O(34)	176.057
H(22)-C(7)	1.091	O(15)-N(14)-O(16)	130.661	C(5)-O(26)-N(32)-O(33)	-4.313
H(21)-C(5)	1.092	O(15)-N(14)-O(13)	111.320	C(7)-O(25)-N(29)-O(31)	-179.441
H(20)-C(4)	1.091	O(16)-N(14)-O(13)	118.004	C(7)-O(25)-N(29)-O(30)	0.988
H(19)-C(2)	1.091	N(38)-O(28)-C(2)	115.277	C(7)-O(25)-N(29)-O(33)	-62.079
O(28)-C(2)	1.445	N(35)-O(27)-C(4)	115.747	C(1)-O(13)-N(14)-O(16)	-8.536
O(27)-C(4)	1.429	N(32)-O(26)-C(5)	115.810	C(1)-O(13)-N(14)-O(15)	172.707
O(26)-C(5)	1.426	N(29)-O(25)-C(7)	116.128	N(38)-O(28)-C(2)-O(3)	-143.545
O(25)-C(7)	1.435	C(1)-O(13)-N(14)	114.926	N(38)-O(28)-C(2)-H(19)	-21.820

Table S2. continuation

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
O(12)-N(10)	1.213	O(12)-N(10)-O(11)	130.600	N(38)-O(28)-C(2)-C(1)	99.975
O(11)-N(10)	1.203	O(12)-N(10)-O(9)	117.002	N(35)-O(27)-C(4)-O(3)	-108.437
N(10)-O(9)	1.429	O(11)-N(10)-O(9)	112.398	N(35)-O(27)-C(4)-C(5)	136.754
O(9)-C(8)	1.436	N(10)-O(9)-C(8)	113.119	N(35)-O(27)-C(4)-H(20)	16.584
C(8)-C(7)	1.524	H(24)-C(8)-H(23)	109.586	N(32)-O(26)-C(5)-C(4)	-113.270
C(7)-O(6)	1.403	H(24)-C(8)-O(9)	111.062	N(32)-O(26)-C(5)-O(6)	131.553
O(6)-C(5)	1.398	H(24)-C(8)-C(7)	110.388	N(32)-O(26)-C(5)-H(21)	7.320
C(5)-C(4)	1.536	H(23)-C(8)-O(9)	110.784	N(29)-O(25)-C(7)-O(6)	117.775
C(4)-O(3)	1.401	H(23)-C(8)-C(7)	109.596	N(29)-O(25)-C(7)-C(8)	-126.154
O(3)-C(2)	1.399	O(9)-C(8)-C(7)	105.353	N(29)-O(25)-C(7)-H(22)	-5.123
		H(22)-C(7)-O(25)	109.446	O(11)-N(10)-O(9)-C(8)	179.976
		H(22)-C(7)-C(8)	112.023	O(12)-N(10)-O(9)-C(8)	-0.005
		H(22)-C(7)-O(6)	111.628	N(10)-O(9)-C(8)-C(7)	-178.053
		O(25)-C(7)-C(8)	106.067	N(10)-O(9)-C(8)-H(23)	-59.614
		O(25)-C(7)-O(6)	109.862	N(10)-O(9)-C(8)-H(24)	62.418
		C(8)-C(7)-O(6)	107.648	O(9)-C(8)-C(7)-O(6)	-67.014
		C(7)-O(6)-C(5)	117.057	O(9)-C(8)-C(7)-O(25)	175.427
		H(21)-C(5)-O(26)	109.726	O(9)-C(8)-C(7)-H(22)	56.072
		H(21)-C(5)-O(6)	112.790	H(23)-C(8)-C(7)-O(6)	173.754
		H(21)-C(5)-C(4)	110.520	H(23)-C(8)-C(7)-O(25)	56.195
		O(26)-C(5)-O(6)	109.402	H(23)-C(8)-C(7)-H(22)	-63.160
		O(26)-C(5)-C(4)	108.091	H(24)-C(8)-C(7)-O(6)	52.961
		O(6)-C(5)-C(4)	106.157	H(24)-C(8)-C(7)-O(25)	-64.597
		H(20)-C(4)-O(27)	110.099	H(24)-C(8)-C(7)-H(22)	176.048
		H(20)-C(4)-C(5)	111.065	C(8)-C(7)-O(6)-C(5)	175.908
		H(20)-C(4)-O(3)	112.198	O(25)-C(7)-O(6)-C(5)	-69.022
		O(27)-C(4)-C(5)	105.942	H(22)-C(7)-O(6)-C(5)	52.580
		O(27)-C(4)-O(3)	111.240	C(7)-O(6)-C(5)-C(4)	176.815

Table S2. continuation

Bond angles [°]		Dihedral angels [°]	
C(5)-C(4)-O(3)	106.054	C(7)-O(6)-C(5)-O(26)	-66.774
C(4)-O(3)-C(2)	117.326	C(7)-O(6)-C(5)-H(21)	55.646
C(1)-C(2)-H(19)	111.588	O(6)-C(5)-C(4)-O(3)	176.265
C(1)-C(2)-O(28)	108.465	O(6)-C(5)-C(4)-O(27)	-65.423
C(1)-C(2)-O(3)	108.092	O(6)-C(5)-C(4)-H(20)	54.115
H(19)-C(2)-O(28)	109.184	O(26)-C(5)-C(4)-O(3)	58.976
H(19)-C(2)-O(3)	112.176	O(26)-C(5)-C(4)-O(27)	177.287
O(28)-C(2)-O(3)	107.177	O(26)-C(5)-C(4)-H(20)	-63.174
		H(21)-C(5)-C(4)-O(3)	-61.117
		H(21)-C(5)-C(4)-O(27)	57.195
		H(21)-C(5)-C(4)-H(20)	176.733
		C(5)-C(4)-O(3)-C(2)	-169.527
		O(27)-C(4)-O(3)-C(2)	75.733
		H(20)-C(4)-O(3)-C(2)	-48.103
		C(4)-O(3)-C(2)-O(28)	67.986
		C(4)-O(3)-C(2)-H(19)	-51.843
		C(4)-O(3)-C(2)-C(1)	-175.288

Table S3. The geometric parameters of TS

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
O(28)-N(38)	1.455	O(9)-N(10)-O(11)	112.049	C(2)-O(28)-N(38)-O(39)	-5.035
O(6)-C(7)	1.951	O(9)-N(10)-O(12)	117.150	C(2)-O(28)-N(38)-O(40)	176.021
H(22)-C(7)	1.093	O(11)-N(10)-O(12)	130.801	C(5)-O(6)-C(7)-H(22)	-169.463
O(25)-N(29)	1.937	O(30)-N(29)-O(31)	142.088	C(5)-O(6)-C(7)-O(25)	71.401
O(39)-N(38)	1.210	O(30)-N(29)-O(25)	110.100	C(5)-O(6)-C(7)-C(8)	-53.675
O(37)-N(35)	1.203	O(31)-N(29)-O(25)	103.366	C(7)-O(25)-N(29)-O(31)	-132.707
O(36)-N(35)	1.207	C(8)-O(9)-N(10)	114.651	C(7)-O(25)-N(29)-O(30)	65.403
N(35)-O(27)	1.446	C(7)-C(8)-O(9)	113.432	O(37)-N(35)-O(27)-C(4)	-175.769
O(34)-N(32)	1.205	C(7)-C(8)-H(23)	107.937	O(36)-N(35)-O(27)-C(4)	3.985
O(33)-N(32)	1.215	C(7)-C(8)-H(24)	110.384	O(34)-N(32)-O(26)-C(5)	-176.580
N(32)-O(26)	1.413	O(9)-C(8)-H(23)	110.588	O(33)-N(32)-O(26)-C(5)	3.529
O(31)-N(29)	1.172	O(9)-C(8)-H(24)	104.751	N(38)-O(28)-C(2)-H(19)	31.913
O(30)-N(29)	1.176	H(23)-C(8)-H(24)	109.716	N(38)-O(28)-C(2)-O(3)	-92.218
O(28)-C(2)	1.428	O(26)-N(32)-O(33)	118.065	N(38)-O(28)-C(2)-C(1)	152.190
O(27)-C(4)	1.426	O(26)-N(32)-O(34)	112.406	N(35)-O(27)-C(4)-H(20)	42.348
O(26)-C(5)	1.477	O(33)-N(32)-O(34)	129.529	N(35)-O(27)-C(4)-C(5)	161.947
O(25)-C(7)	1.258	C(7)-O(25)-N(29)	99.488	N(35)-O(27)-C(4)-O(3)	-82.160
H(24)-C(8)	1.089	O(40)-N(38)-O(39)	130.913	N(32)-O(26)-C(5)-H(21)	-47.811
H(23)-C(8)	1.095	O(40)-N(38)-O(28)	111.553	N(32)-O(26)-C(5)-O(6)	76.740
O(40)-N(38)	1.197	O(39)-N(38)-O(28)	117.523	N(32)-O(26)-C(5)-C(4)	-160.544
H(21)-C(5)	1.101	O(27)-N(35)-O(36)	117.731	N(29)-O(25)-C(7)-O(6)	34.722
H(20)-C(4)	1.091	O(27)-N(35)-O(37)	111.638	N(29)-O(25)-C(7)-H(22)	-51.367
H(19)-C(2)	1.090	O(36)-N(35)-O(37)	130.630	N(29)-O(25)-C(7)-C(8)	156.810
H(18)-C(1)	1.091	C(5)-O(26)-N(32)	115.384	O(16)-N(14)-O(13)-C(1)	-16.447
H(17)-C(1)	1.092	O(13)-N(14)-O(15)	111.343	O(15)-N(14)-O(13)-C(1)	165.252
O(16)-N(14)	1.208	O(13)-N(14)-O(16)	118.169	N(14)-O(13)-C(1)-H(18)	27.084
O(15)-N(14)	1.204	O(15)-N(14)-O(16)	130.461	N(14)-O(13)-C(1)-H(17)	146.101
N(14)-O(13)	1.445	C(8)-C(7)-O(25)	116.967	N(14)-O(13)-C(1)-C(2)	-95.156
O(13)-C(1)	1.429	C(8)-C(7)-H(22)	116.978	O(12)-N(10)-O(9)-C(8)	1.228

Table S3. continuation

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
O(12)-N(10)	1.213	C(8)-C(7)-O(6)	112.681	O(11)-N(10)-O(9)-C(8)	-178.798
O(11)-N(10)	1.200	O(25)-C(7)-H(22)	120.000	N(10)-O(9)-C(8)-H(24)	160.605
N(10)-O(9)	1.440	O(25)-C(7)-O(6)	100.209	N(10)-O(9)-C(8)-H(23)	42.469
O(9)-C(8)	1.430	H(22)-C(7)-O(6)	81.561	N(10)-O(9)-C(8)-C(7)	-78.954
C(8)-C(7)	1.515	N(38)-O(28)-C(2)	115.563	H(24)-C(8)-C(7)-O(6)	76.874
O(6)-C(5)	1.344	C(4)-O(27)-N(35)	114.465	H(24)-C(8)-C(7)-H(22)	168.837
C(5)-C(4)	1.555	C(1)-O(13)-N(14)	114.746	H(24)-C(8)-C(7)-O(25)	-38.477
C(4)-O(3)	1.402	C(5)-O(6)-C(7)	140.437	H(23)-C(8)-C(7)-O(6)	-163.221
O(3)-C(2)	1.404	C(4)-C(5)-O(6)	116.493	H(23)-C(8)-C(7)-H(22)	-71.258
C(2)-C(1)	1.533	C(4)-C(5)-H(21)	108.385	H(23)-C(8)-C(7)-O(25)	81.428
		C(4)-C(5)-O(26)	99.278	O(9)-C(8)-C(7)-O(6)	-40.325
		O(6)-C(5)-H(21)	113.937	O(9)-C(8)-C(7)-H(22)	51.639
		O(6)-C(5)-O(26)	110.001	O(9)-C(8)-C(7)-O(25)	-155.676
		H(21)-C(5)-O(26)	107.464	C(7)-O(6)-C(5)-O(26)	166.482
		O(3)-C(4)-C(5)	108.474	C(7)-O(6)-C(5)-H(21)	-72.788
		O(3)-C(4)-H(20)	112.685	C(7)-O(6)-C(5)-C(4)	54.573
		O(3)-C(4)-O(27)	109.244	O(26)-C(5)-C(4)-O(27)	-179.357
		C(5)-C(4)-H(20)	111.135	O(26)-C(5)-C(4)-H(20)	-60.194
		C(5)-C(4)-O(27)	104.468	O(26)-C(5)-C(4)-O(3)	64.215
		H(20)-C(4)-O(27)	110.488	H(21)-C(5)-C(4)-O(27)	68.635
		C(2)-O(3)-C(4)	119.603	H(21)-C(5)-C(4)-H(20)	-172.202
		C(1)-C(2)-O(3)	107.603	H(21)-C(5)-C(4)-O(3)	-47.793
		C(1)-C(2)-H(19)	112.209	O(6)-C(5)-C(4)-O(27)	-61.409
		C(1)-C(2)-O(28)	103.703	O(6)-C(5)-C(4)-H(20)	57.753
		O(3)-C(2)-H(19)	111.211	O(6)-C(5)-C(4)-O(3)	-177.838
		O(3)-C(2)-O(28)	111.689	O(27)-C(4)-O(3)-C(2)	119.454

Table S3. continuation

Bond angles [°]		Dihedral angles [°]	
H(19)-C(2)-O(28)	110.187	H(20)-C(4)-O(3)-C(2)	-3.758
C(2)-C(1)-O(13)	109.230	C(5)-C(4)-O(3)-C(2)	-127.241
C(2)-C(1)-H(17)	110.348	C(4)-O(3)-C(2)-O(28)	100.014
C(2)-C(1)-H(18)	110.713	C(4)-O(3)-C(2)-H(19)	-23.539
O(13)-C(1)-H(17)	105.733	C(4)-O(3)-C(2)-C(1)	-146.804
O(13)-C(1)-H(18)	110.826	O(28)-C(2)-C(1)-H(18)	55.454
H(17)-C(1)-H(18)	109.876	O(28)-C(2)-C(1)-H(17)	-66.411
		O(28)-C(2)-C(1)-O(13)	177.762
		H(19)-C(2)-C(1)-H(18)	174.349
		H(19)-C(2)-C(1)-H(17)	52.484
		H(19)-C(2)-C(1)-O(13)	-63.343
		O(3)-C(2)-C(1)-H(18)	-63.000
		O(3)-C(2)-C(1)-H(17)	175.136
		O(3)-C(2)-C(1)-O(13)	59.308

Table S4. The geometric parameters of products

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
O(6)-C(7)	3.324	O(36)-N(35)-O(37)	130.726	C(5)-O(6)-C(7)-O(25)	32.458
N(29)-O(25)	3.300	O(15)-N(14)-O(16)	130.650	C(5)-O(6)-C(7)-H(22)	123.969
O(26)-C(5)	3.224	O(30)-N(29)-O(31)	134.727	C(5)-O(6)-C(7)-C(8)	-118.635
O(39)-N(38)	1.211	O(30)-N(29)-O(25)	136.292	O(31)-N(29)-O(25)-C(7)	-52.913
N(38)-O(28)	1.437	O(31)-N(29)-O(25)	63.801	O(30)-N(29)-O(25)-C(7)	178.748
O(37)-N(35)	1.197	C(7)-O(25)-N(29)	146.834	N(32)-O(26)-C(5)-O(6)	-54.689
O(36)-N(35)	1.212	O(9)-N(10)-O(11)	112.714	N(32)-O(26)-C(5)-C(4)	65.772
O(34)-N(32)	1.205	O(9)-N(10)-O(12)	116.901	O(39)-N(38)-O(28)-C(2)	-12.325
O(33)-N(32)	1.445	O(11)-N(10)-O(12)	130.384	O(40)-N(38)-O(28)-C(2)	169.069
N(32)-O(26)	1.203	O(6)-C(7)-C(8)	105.859	O(34)-N(32)-O(26)-C(5)	-13.685
O(31)-N(29)	1.187	O(6)-C(7)-H(22)	28.358	O(33)-N(32)-O(26)-C(5)	170.314
O(30)-N(29)	1.192	O(6)-C(7)-O(25)	125.401	N(38)-O(28)-C(2)-H(19)	-25.810
O(28)-C(2)	1.455	C(8)-C(7)-H(22)	116.789	N(38)-O(28)-C(2)-O(3)	-147.425
O(27)-C(4)	1.426	C(8)-C(7)-O(25)	121.877	N(38)-O(28)-C(2)-C(1)	96.212
O(25)-C(7)	1.210	H(22)-C(7)-O(25)	121.331	N(29)-O(25)-C(7)-H(22)	-71.016
H(24)-C(8)	1.093	C(7)-C(8)-O(9)	112.785	N(29)-O(25)-C(7)-C(8)	109.554
H(23)-C(8)	1.096	C(7)-C(8)-H(23)	109.369	N(29)-O(25)-C(7)-O(6)	-37.245
H(22)-C(7)	1.107	C(7)-C(8)-H(24)	110.405	O(12)-N(10)-O(9)-C(8)	-0.753
O(40)-N(38)	1.202	O(9)-C(8)-H(23)	102.800	O(11)-N(10)-O(9)-C(8)	178.856
H(20)-C(4)	1.092	O(9)-C(8)-H(24)	111.945	N(10)-O(9)-C(8)-H(24)	-55.960
H(19)-C(2)	1.091	H(23)-C(8)-H(24)	109.220	N(10)-O(9)-C(8)-H(23)	-173.057
H(18)-C(1)	1.091	C(8)-O(9)-N(10)	113.014	N(10)-O(9)-C(8)-C(7)	69.277
H(17)-C(1)	1.093	O(26)-N(32)-O(33)	118.683	H(24)-C(8)-C(7)-O(25)	-40.036
O(16)-N(14)	1.209	O(26)-N(32)-O(34)	130.779	H(24)-C(8)-C(7)-H(22)	140.509
O(15)-N(14)	1.201	O(33)-N(32)-O(34)	110.439	H(24)-C(8)-C(7)-O(6)	112.319
O(13)-C(1)	1.430	C(7)-O(6)-C(5)	116.568	H(23)-C(8)-C(7)-O(25)	80.169
O(12)-N(10)	1.216	O(40)-N(38)-O(28)	111.835	H(23)-C(8)-C(7)-H(22)	-99.286
O(11)-N(10)	1.200	O(40)-N(38)-O(39)	130.650	H(23)-C(8)-C(7)-O(6)	-127.477

Table S4. continuation

Bond lengths [Å]		Bond angles [°]		Dihedral angles [°]	
N(10)-O(9)	1.429	O(28)-N(38)-O(39)	117.497	O(9)-C(8)-C(7)-O(25)	-166.104
O(9)-C(8)	1.434	N(32)-O(26)-C(5)	109.543	O(9)-C(8)-C(7)-H(22)	14.441
C(8)-C(7)	1.523	C(2)-O(28)-N(38)	115.489	O(9)-C(8)-C(7)-O(6)	-13.749
O(6)-C(5)	1.206	C(4)-C(5)-O(6)	121.038	C(7)-O(6)-C(5)-O(26)	-15.632
C(5)-C(4)	1.541	C(4)-C(5)-O(26)	83.701	C(7)-O(6)-C(5)-C(4)	-106.266
C(4)-O(3)	1.404	O(6)-C(5)-O(26)	103.338	O(26)-C(5)-C(4)-O(27)	-163.630
O(3)-C(2)	1.395	O(3)-C(4)-C(5)	107.124	O(26)-C(5)-C(4)-H(20)	-45.120
C(2)-C(1)	1.524	O(3)-C(4)-H(20)	112.183	O(26)-C(5)-C(4)-O(3)	76.765
		O(3)-C(4)-O(27)	111.963	O(6)-C(5)-C(4)-O(27)	-61.832
		C(5)-C(4)-H(20)	109.500	O(6)-C(5)-C(4)-H(20)	56.677
		C(5)-C(4)-O(27)	105.813	O(6)-C(5)-C(4)-O(3)	178.563
		H(20)-C(4)-O(27)	109.995	O(27)-C(4)-O(3)-C(2)	90.003
		C(2)-O(3)-C(4)	117.616	H(20)-C(4)-O(3)-C(2)	-34.233
		C(1)-C(2)-O(3)	108.386	C(5)-C(4)-O(3)-C(2)	-154.421
		C(1)-C(2)-H(19)	111.941	C(4)-O(3)-C(2)-O(28)	70.598
		C(1)-C(2)-O(28)	108.601	C(4)-O(3)-C(2)-H(19)	-48.363
		O(3)-C(2)-H(19)	112.802	C(4)-O(3)-C(2)-C(1)	-172.895
		O(3)-C(2)-O(28)	106.164	O(28)-C(2)-C(1)-H(18)	59.861
		H(19)-C(2)-O(28)	108.714	O(28)-C(2)-C(1)-H(17)	-61.760
		C(2)-C(1)-O(13)	110.104	O(28)-C(2)-C(1)-O(13)	-177.045
		C(2)-C(1)-H(17)	109.445	H(19)-C(2)-C(1)-H(18)	179.896
		C(2)-C(1)-H(18)	110.445	H(19)-C(2)-C(1)-H(17)	58.276
		O(13)-C(1)-H(17)	105.295	H(19)-C(2)-C(1)-O(13)	-57.010
		O(13)-C(1)-H(18)	111.124	O(3)-C(2)-C(1)-H(18)	-55.062
		H(17)-C(1)-H(18)	110.301	O(3)-C(2)-C(1)-H(17)	-176.682
				O(3)-C(2)-C(1)-O(13)	68.033

Received: June 27, 2018

First published online: June 27, 2019