

Table 6 (deposited) Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) of H-atoms at 1.0 GPa, 2.0 GPa, 3.0 GPa, 4.0 GPa (1st, 2nd, 3rd, 4th lines downwards)

$$U_{\text{eq}} = (1/3) \sum_i \sum_j U^{ij} \alpha^i \alpha^j a_i a_j$$

Atom H (coresponding non-H-atom)	x	y	z	Ueq
H1' (OH)	0.071 (5)	0.981 (5)	0.240 (3)	0.060
	0.053 (4)	0.985 (4)	0.246 (3)	0.047
	0.051 (4)	1.001 (4)	0.240 (3)	0.044
	0.042 (5)	1.013 (4)	0.243 (3)	0.040
H2 (C2)	-0.161 (4)	0.896 (2)	0.0704 (5)	0.046
	-0.172 (4)	0.897 (2)	0.0719 (5)	0.030
	-0.177 (4)	0.8982 (19)	0.0751 (6)	0.030
	-0.190 (4)	0.898 (2)	0.0833 (7)	0.021
H3 (C3)	-0.181 (3)	0.7307 (3)	-0.0907 (12)	0.038
	-0.194 (3)	0.7270 (3)	-0.0883 (12)	0.044
	-0.202 (3)	0.7265 (3)	-0.0863 (11)	0.038
	-0.228 (4)	0.7217 (5)	-0.0740 (12)	0.032
H5 (C5)	0.356 (3)	0.586 (2)	0.0026 (5)	0.030
	0.366 (3)	0.587 (2)	0.0011 (5)	0.033
	0.369 (3)	0.5923 (19)	-0.0001 (5)	0.030
	0.375 (4)	0.614 (2)	-0.0047 (7)	0.023
H6 (C6)	0.398 (3)	0.7474 (3)	0.1607 (12)	0.039
	0.397 (3)	0.7587 (3)	0.1601 (10)	0.023
	0.402 (3)	0.7677 (3)	0.1606 (10)	0.023
	0.405 (4)	0.7891 (4)	0.1541 (13)	0.026
H2' (N)	-0.080 (5)	0.5317 (6)	-0.1893 (10)	0.039
	-0.078 (4)	0.5306 (5)	-0.1909 (9)	0.024
	-0.091 (4)	0.5305 (4)	-0.1916 (9)	0.025
	-0.125 (6)	0.543 (3)	-0.179 (3)	0.029
H8A (C8)	-0.045 (2)	0.419 (3)	-0.3430 (14)	0.085
	0.153 (2)	0.409 (2)	-0.3889 (11)	0.061
	0.088 (4)	0.2680 (16)	-0.3087 (8)	0.068
	0.134 (3)	0.417 (2)	-0.3720 (12)	0.053
H8B (C8)	0.101 (4)	0.2917 (17)	-0.3110 (11)	0.085
	-0.052 (2)	0.416 (2)	-0.3472 (12)	0.061
	0.150 (2)	0.407 (2)	-0.3870 (11)	0.068
	-0.063 (2)	0.383 (2)	-0.3223 (10)	0.053
H8C (C8)	0.149 (2)	0.420 (2)	-0.3893 (13)	0.085
	0.089 (4)	0.2756 (16)	-0.3101 (8)	0.061
	-0.058 (2)	0.412 (2)	-0.3441 (11)	0.068
	0.118 (4)	0.259 (2)	-0.2993 (9)	0.053