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Mass Spectrometry of 1,2,5-Oxadiazole *N*-Oxide Derivatives. Use of Deuterated Analogues in Fragmentation Pattern Studies

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Interatomic bond distances (Å) and some selected angles (°) for derivative **6-d_1**.

Bond distances		Bond angles	
O(1)-N(1)	1.237(2)	N(2)-O(2)-N(1)	107.13(17)
O(2)-N(2)	1.371(3)	O(1)-N(1)-C(1)	134.4(3)
O(2)-N(1)	1.434(3)	O(1)-N(1)-O(2)	117.3(2)
N(1)-C(1)	1.316(3)	C(1)-N(1)-O(2)	108.26(19)
N(2)-C(2)	1.311(3)	C(2)-N(2)-O(2)	107.1(2)
C(1)-C(2)	1.413(3)	N(1)-C(1)-C(2)	106.2(2)
C(1)-C(17)	1.486(3)	N(1)-C(1)-C(17)	121.3(2)
C(2)-C(21)	1.468(3)	C(2)-C(1)-C(17)	132.1(2)
N(11)-C(16)	1.452(3)	N(2)-C(2)-C(1)	111.4(2)
N(11)-C(17)	1.458(3)	N(2)-C(2)-C(21)	119.6(2)
N(11)-C(12)	1.458(3)	C(1)-C(2)-C(21)	129.0(2)
C(12)-C(13)	1.498(3)	C(16)-N(11)-C(17)	110.8(2)
C(13)-N(14)	1.442(3)	C(16)-N(11)-C(12)	109.44(19)
N(14)-C(15)	1.439(4)	C(17)-N(11)-C(12)	111.54(19)
N(14)-C(18)	1.460(3)	N(11)-C(12)-C(13)	110.3(2)
C(15)-C(16)	1.508(4)	N(14)-C(13)-C(12)	111.2(2)
C(21)-C(26)	1.384(3)	C(15)-N(14)-C(13)	109.0(2)
C(21)-C(22)	1.386(3)	C(15)-N(14)-C(18)	111.6(2)
C(22)-C(23)	1.377(3)	C(13)-N(14)-C(18)	111.1(2)
C(23)-C(24)	1.368(4)	N(14)-C(15)-C(16)	110.9(2)
C(24)-C(25)	1.368(4)	N(11)-C(16)-C(15)	110.9(2)
C(25)-C(26)	1.376(3)	N(11)-C(17)-C(1)	113.78(19)
	C(26)-C(21)-C(2)	119.7(2)	
	C(22)-C(21)-C(2)	120.7(2)	

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Anisotropic displacement parameters ($Å^2$ x 10^3) for **6-d_1**. The anisotropic displacement factor exponent takes the form: $-2\delta^2(h^2a^{*2}U_{11} + + 2hka^*b^*U_{12})$.

Atom	U11	U22	U33	U23	U13	U12
O(1)	147(2)	91(1)	51(1)	-2(1)	33(1)	21(1)
O(2)	108(2)	82(1)	81(1)	3(1)	52(1)	9(1)
N(1)	108(2)	61(1)	55(1)	-2(1)	32(1)	12(1)
N(2)	86(2)	72(1)	71(1)	0(1)	37(1)	2(1)
C(1)	78(2)	49(1)	49(1)	1(1)	20(1)	7(1)
C(2)	68(2)	45(1)	61(1)	-1(1)	25(1)	2(1)
N(11)	65(1)	61(1)	51(1)	5(1)	12(1)	-7(1)
C(12)	76(2)	74(2)	65(2)	18(1)	24(1)	10(1)
C(13)	73(2)	76(2)	73(2)	12(1)	24(1)	4(1)
N(14)	62(1)	86(2)	71(1)	-1(1)	10(1)	-4(1)
C(15)	86(2)	104(2)	108(2)	11(2)	45(2)	-13(2)
C(16)	87(2)	81(2)	87(2)	18(2)	24(2)	-14(2)
C(17)	83(2)	54(1)	55(1)	3(1)	9(1)	-2(1)
C(18)	72(2)	115(3)	108(2)	-3(2)	31(2)	5(2)
C(21)	62(1)	46(1)	50(1)	-2(1)	14(1)	-7(1)
C(22)	67(2)	62(1)	59(2)	0(1)	20(1)	1(1)
C(23)	94(2)	71(2)	66(2)	-2(1)	35(2)	-2(1)
C(24)	110(2)	73(2)	52(2)	-3(1)	25(2)	-14(2)
C(25)	74(2)	78(2)	64(2)	8(1)	2(1)	-7(1)
C(26)	64(2)	64(2)	69(2)	1(1)	17(1)	-2(1)

Hydrogen coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **6-d_1**.

Atom	x	y	z	U(eq)
H(12A)	2610	370	7942	88
H(12B)	3791	1038	8863	88
H(13A)	4672	-388	8690	92
H(13B)	3976	-328	6981	92
H(15A)	4745	766	5757	117
H(15B)	5926	1437	6668	117
H(16A)	4550	2171	7585	107
H(16B)	3850	2199	5874	107
H(17A)	1805	2450	6027	85
H(17B)	2376	2316	7719	85
H(18A)	6876	-533	8719	151
H(18B)	7322	166	7825	151
H(18C)	6170	-544	7009	151
H(22)	1067	938	4065	78
H(23)	591	922	1614	92
H(24)	-1492	1372	-84	98
H(25)	-3108	1871	646	97
H(26)	-2661	1897	3088	83