

Contents

1. Sample Information	5
2. Molecular Structure Identification	6
2.1 Test Methods	6
2.2 Test Conditions and Results	7
2.2.1 XRF	7
2.2.1.1 Instrument	7
2.2.1.2 Procedure	7
2.2.1.3. Results	7
2.2.2 XRD	9
2.2.2.1 Instrument	9
2.2.2.2 Procedure	9
2.2.2.3 Results	10
2.2.3 IR	11
2.2.3.1 Instrument	11
2.2.3.2 Procedure	11
2.2.3.3 Results	11
2.2.4 NMR	13
2.2.4.1 Instrument	13
2.2.4.2 Procedure	13
2.2.4.3 Results	13
2.2.5 TEM	15
2.2.5.1 Instrument	15
2.2.5.2 Procedure	15
2.2.5.3 Results	15
2.2.6 SEM	17
2.2.6.1 Instrument	17
2.2.6.2 Procedure	17
2.2.6.3 Results	17

3. Purity Assessment	19
3.1 Test Methods	19
3.2 Test Conditions and Results	20
3.2.1 ICP-AES	20
3.2.1.1 Instrument	20
3.2.1.2 Procedure	20
3.2.3.3 Results	20
4. Impurity Determination	22
4.1 Test Methods	22
4.2 Test Conditions and Results	23
4.2.1 Elemental analysis (EA)	23
4.2.1.1 Instrument	23
4.2.1.2 Procedure	23
4.2.1.3 Results	23
4.2.2 EDS	25
4.2.2.1 Instrument	25
4.2.2.2 Procedure	25
4.2.2.3 Results	26
4.2.3 ICP-MS	28
4.2.3.1 Instrument	28
4.2.3.2 Procedure	28
4.2.3.3 Results	28
4.2.4 Moisture analysis (Karl Fischer titration)	30
4.2.4.1 Instrument	30
4.2.4.2 Procedure	30
4.2.4.3 Results	31
5. Composition Summary	32
6. Authorship of data	33