Electronic Supplementary Information for *Dalton Transactions*
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Electronic Supporting Information

First Example of a Molecular Ce(III) Phosphonate. Synthesis, Structural Characterization and Catalytic activity of $[Ce_2\{Ph_3CPO_2(OEt)\}_4(NO_3)_2(H_2O)_4]$. Structural Diversity of $Ph_3CPO_3H_2$

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Figure S1(a). Asymmetric unit of **1a**

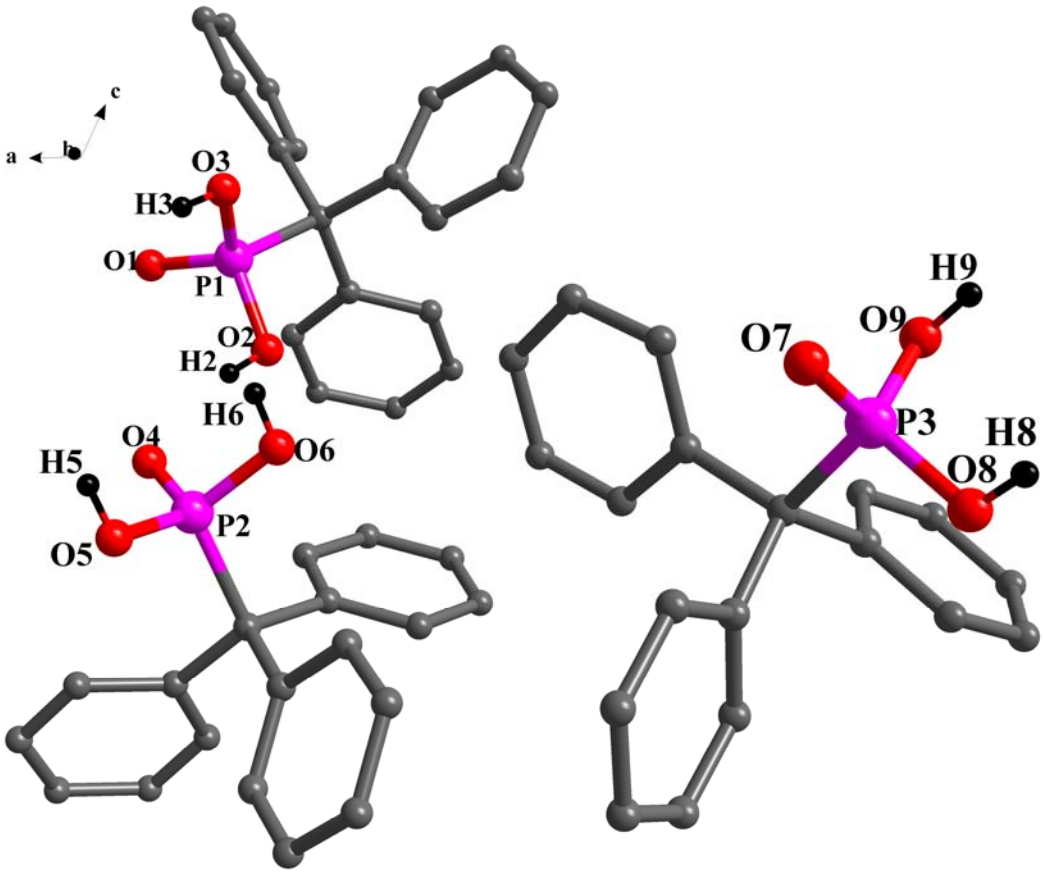

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Figure S1(b). Asymmetric unit of **1b**

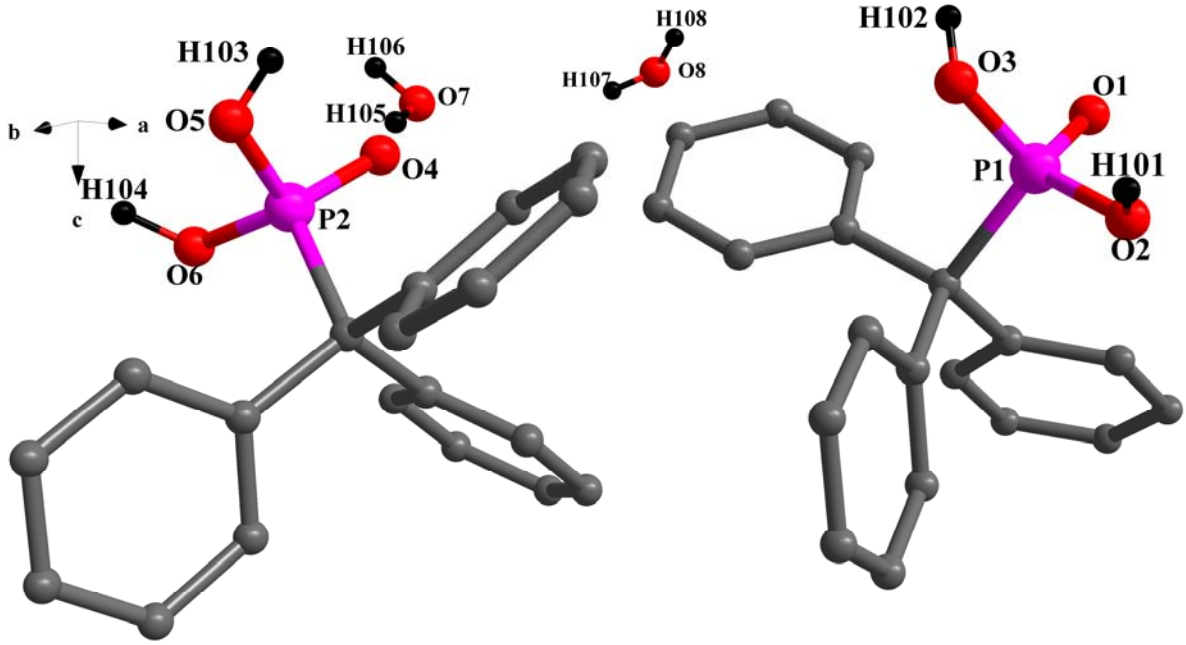

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Figure S1(c). Asymmetric unit of **1c**

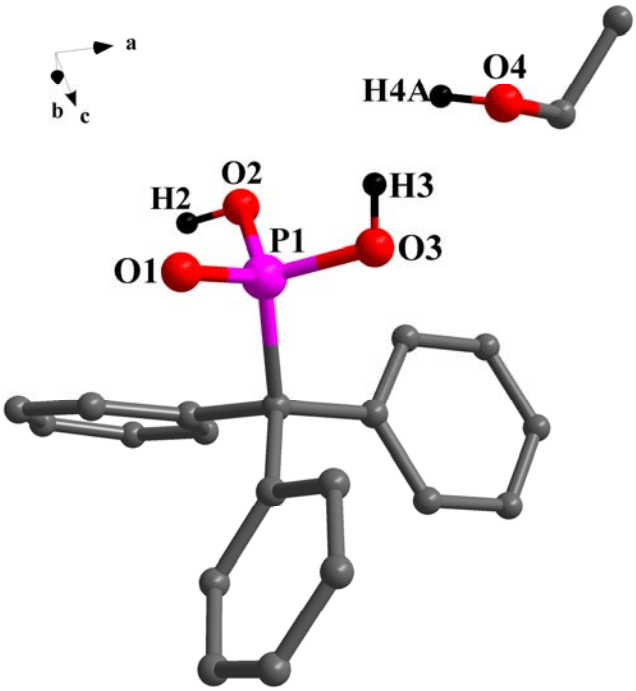

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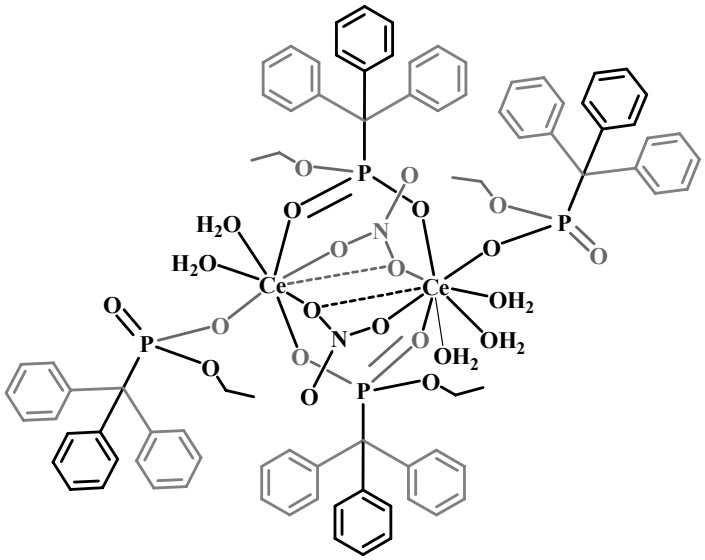
Figure S2(a). ESI-MS of **2**



Formula: $C_{84}H_{91}Ce_2N_2O_{23}P_4$ (Calculated from Sheffield chemputer)

mass	%	
1895	0.4	
1896	0.4	
1897	0.8	
1898	0.6	
1899	100.0	_____
1900	93.1	_____
1901	72.6	_____
1902	40.9	_____
1903	18.5	_____
1904	7.1	_____
1905	2.2	_
1906	0.6	
1907	0.1	
1908	0.0	

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Experimental

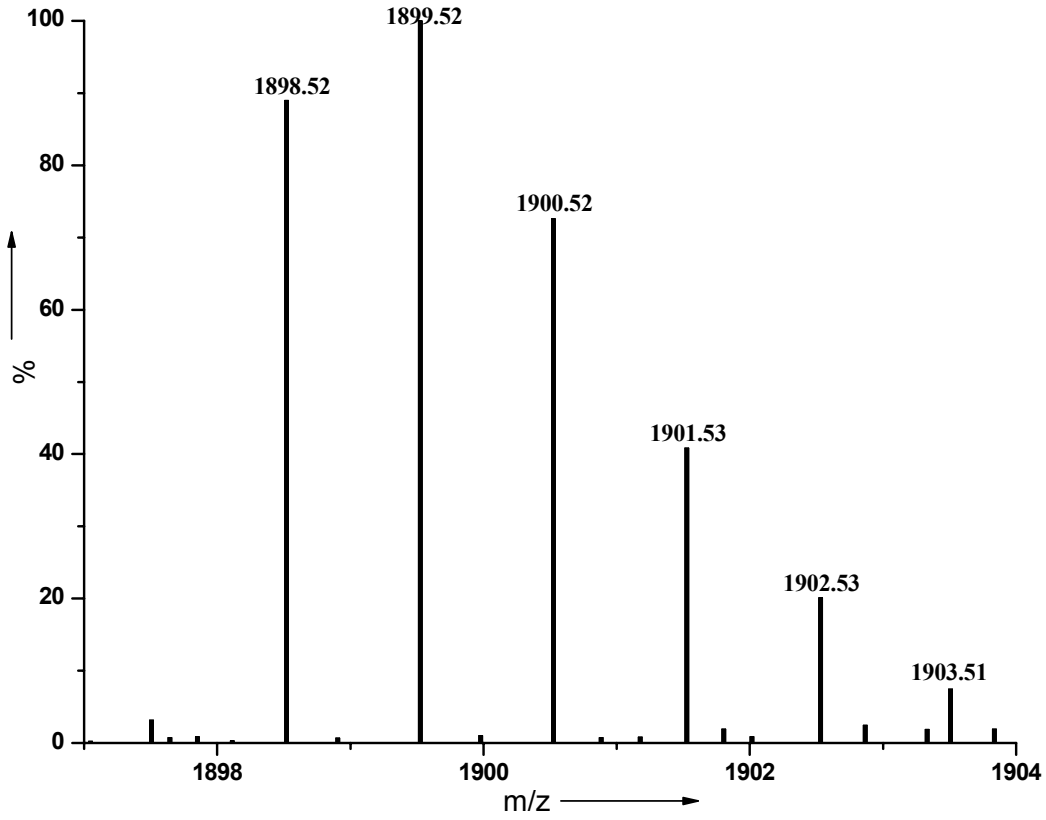

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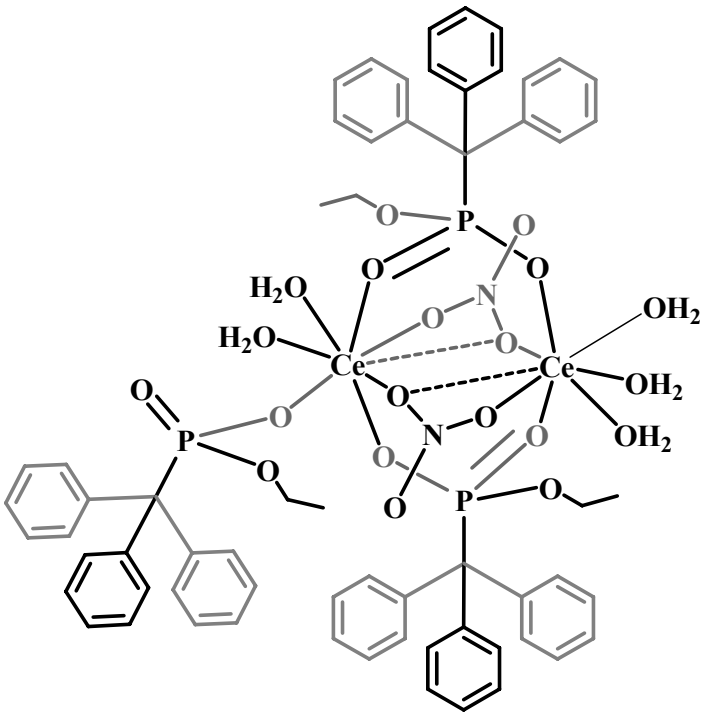
Figure S2(b). ESI-MS of **2** of fragment species



Formula: $C_{63}H_{70}Ce_2N_2O_{20}P_3$ (Calculated from Sheffield chemputer)

```
mass  %
1543   0.4
1544   0.3
1545   0.7
1546   0.5
1547 100.0 ____________________________________________________________
1548  70.2 ____________________________________
1549  53.5 ____________________________
1550  26.0 _____________
1551  10.7 ______
1552   3.6 __
1553   1.0
1554   0.2
1555   0.1
1556   0.0
```

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Experimental

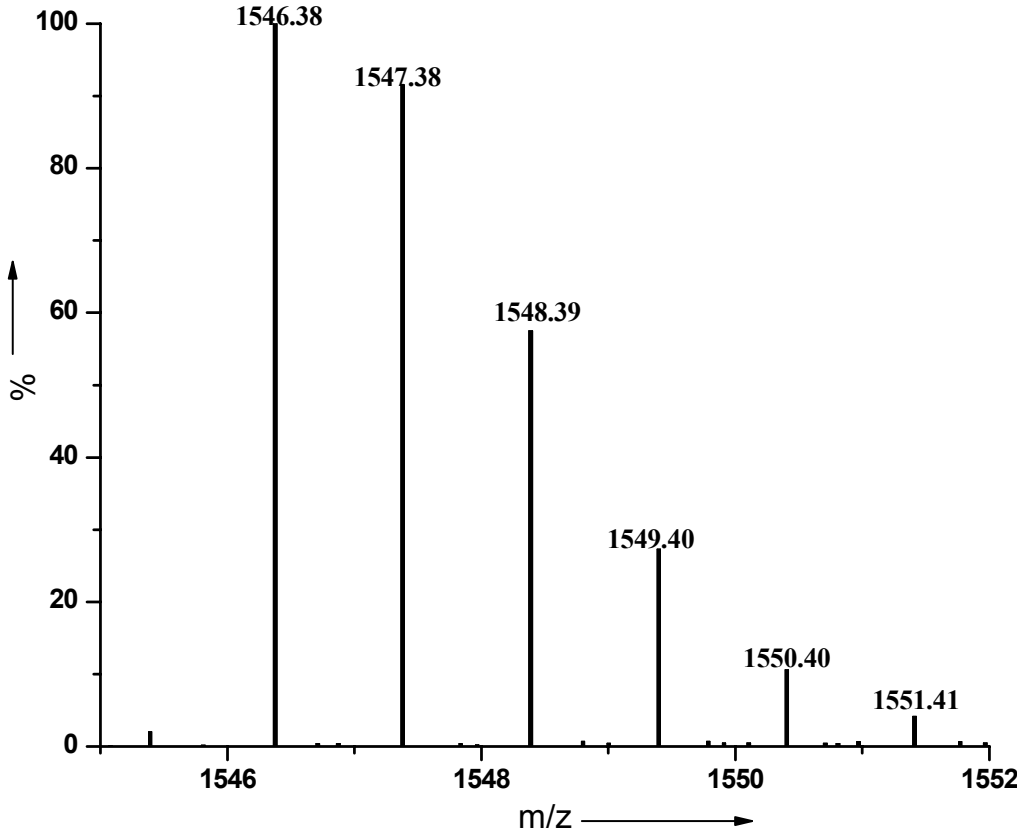

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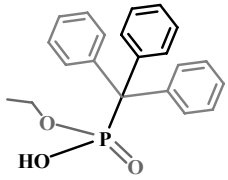
Figure S2(c). ESI-MS of **2** of fragment species



Formula: $C_{21}H_{22}O_3P_1$ (Calculated from Sheffield chemputer)

```
mass  %
353 100.0 ____________________________________________________
354  23.0 ____________
355   3.2 __
356   0.3
357   0.0
```

Experimental

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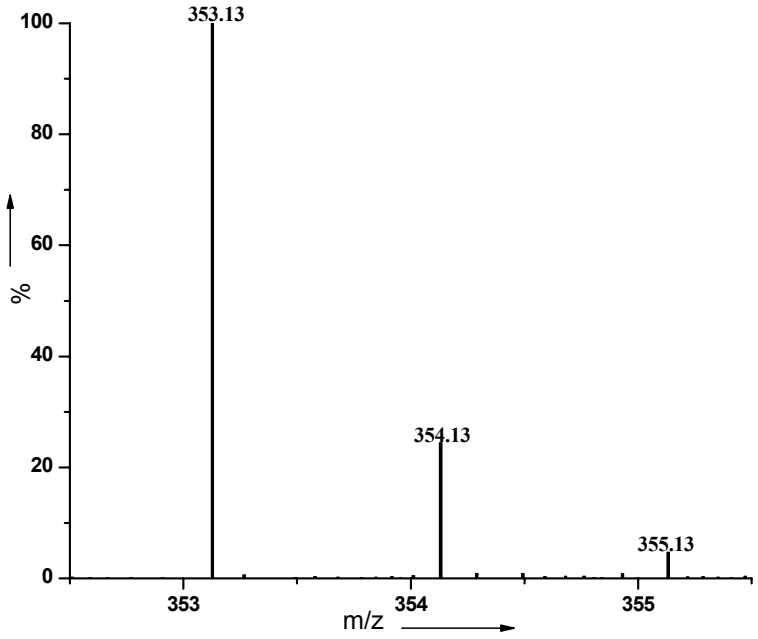
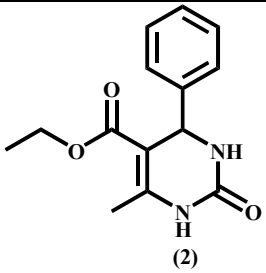


Figures S3-S5. ESI-MS of **3-5**

Compound	(Calculated from Sheffield chemputer), M+H amu
 **(2)**	Formula: $C_{14}H_{17}N_2O_3$ mass % 261 100.0 _____ 262 16.2 _____ 263 1.9 _ 264 0.2 265 0.0

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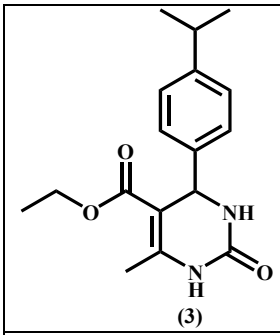
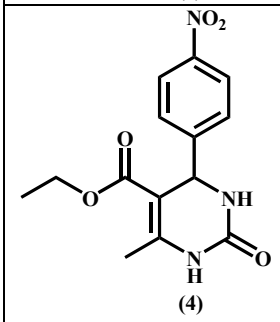


(3)

Formula: $C_{17}H_{23}N_2O_3$

mass %
303 100.0 _____
304 19.5 _____
305 2.4 _
306 0.2
307 0.0



(4)

Formula: $C_{14}H_{16}N_3O_5$

mass %
306 100.0 _____
307 16.6 _____
308 2.3 _
309 0.2
310 0.0

Figure S3. ESI-MS of **3 (Experimental)**

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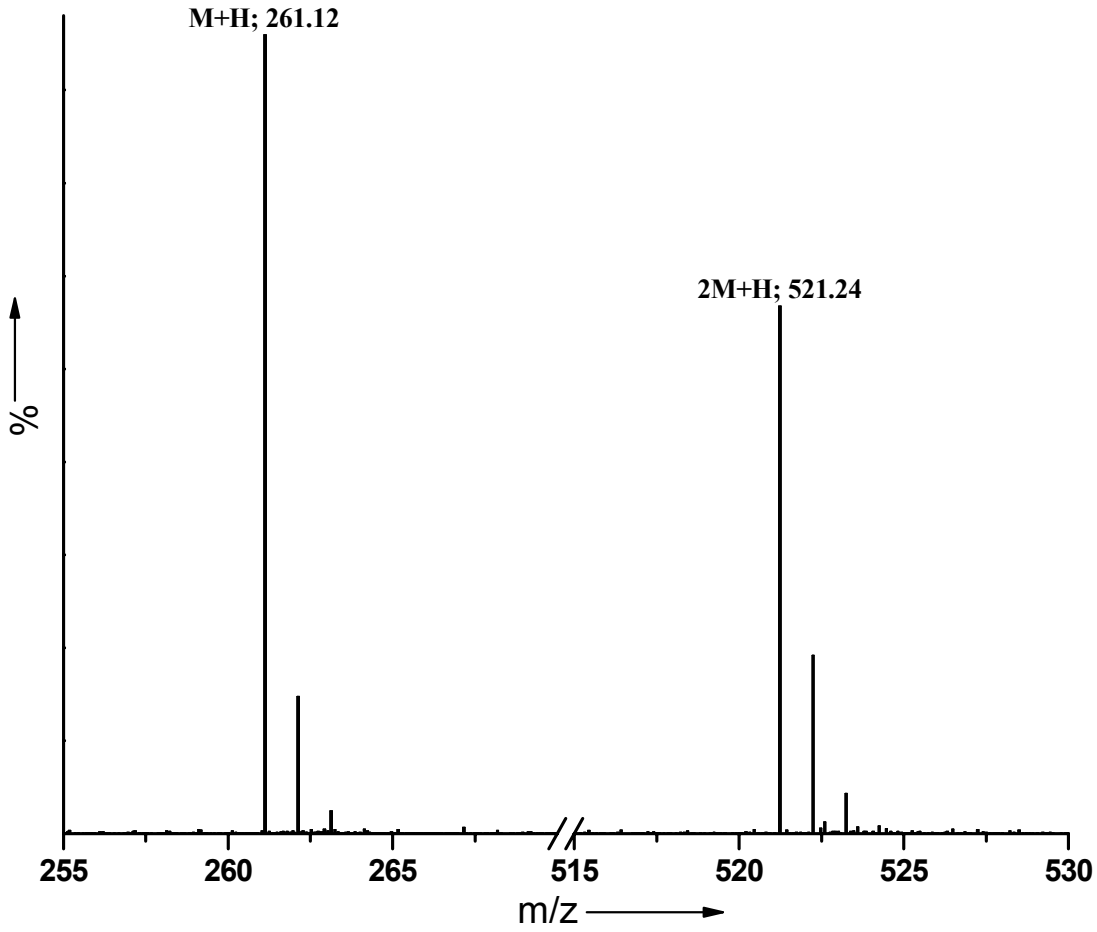

Figure S4. ESI-MS of **4 (Experimental)**

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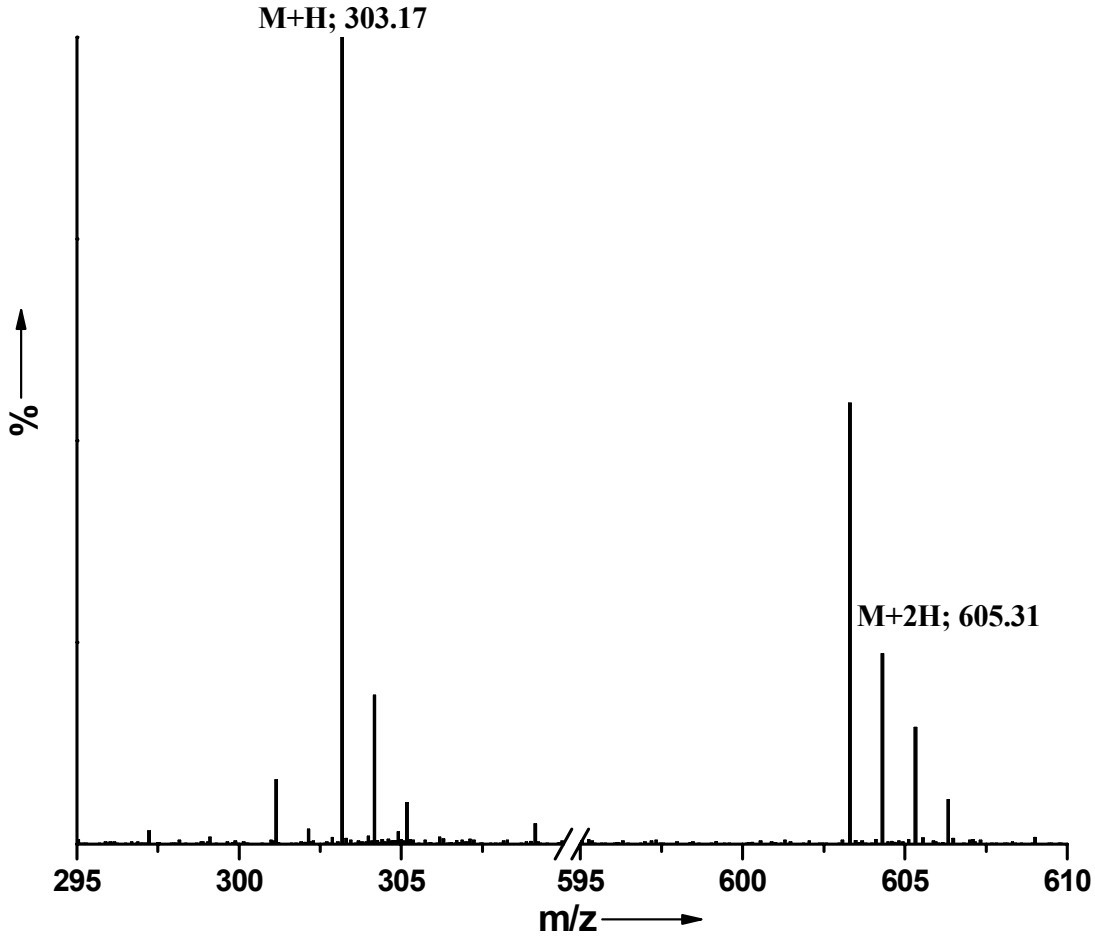

Figure S5. ESI-MS of **5 (Experimental)**

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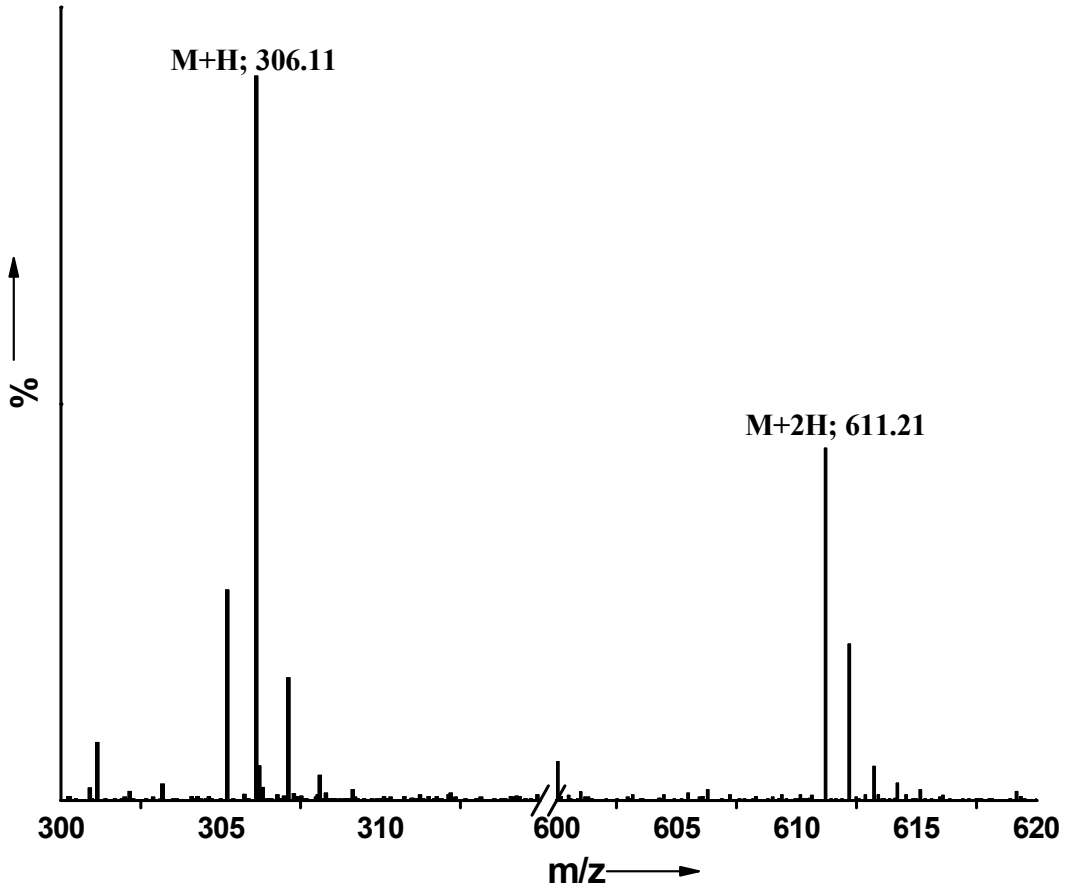

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Figure S6. ^{1}H NMR of **3**

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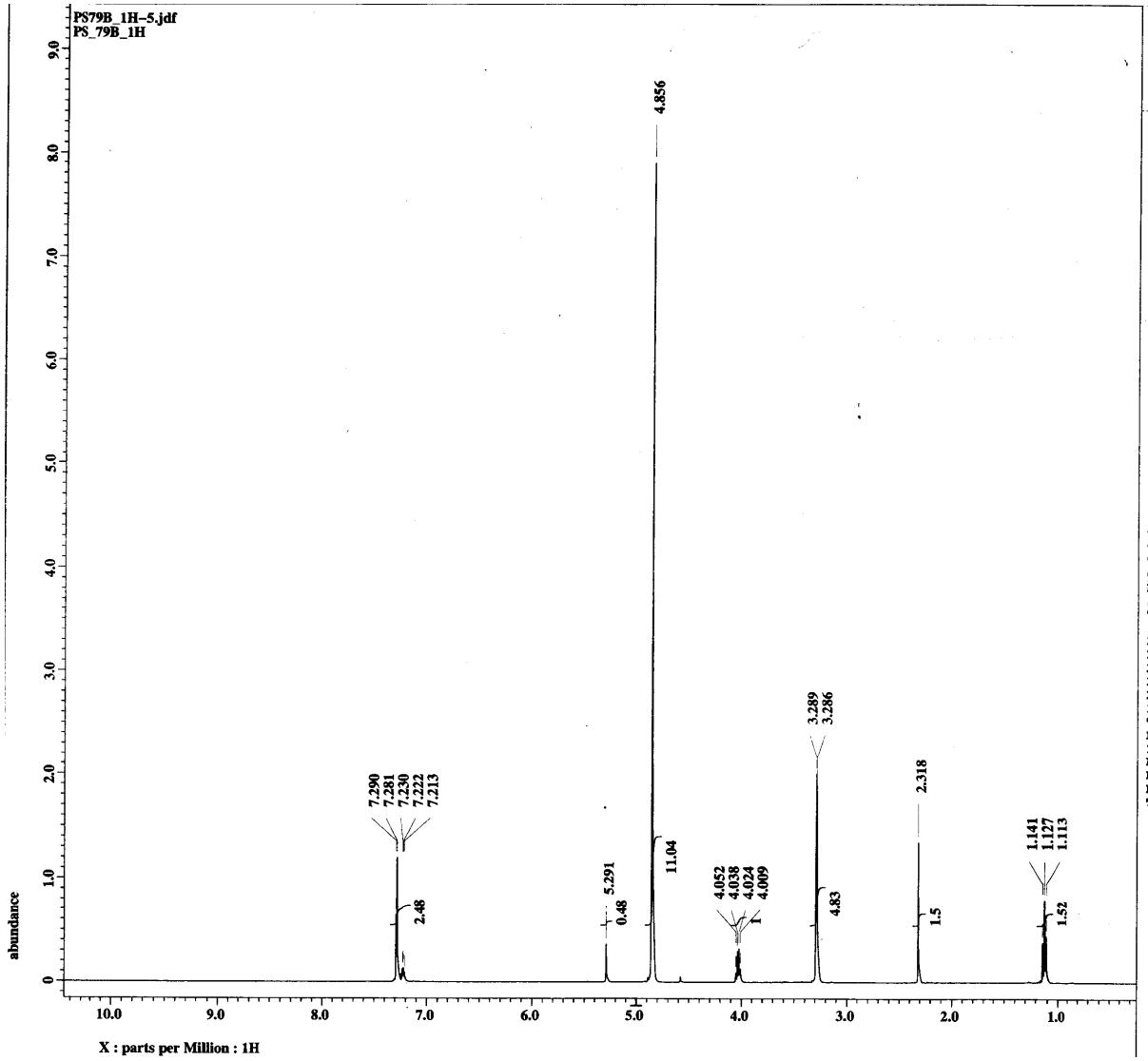

JEOL

Filename	= PS79B_1H-5.jdf
Author	= N.Ahmed
Experiment	= single_pulse.ex2
Sample_id	= PS79B_1H
Solvent	= METHANOL-D3
Creation_time	= 5-FEB-2008 13:54:47
Revision_time	= 5-FEB-2008 13:57:56
Current_time	= 5-FEB-2008 13:58:02
Comment	= PS_79B_1H
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 3.49175808[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 32768
X_prescans	= 1
X_resolution	= 0.28638868[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.25[us]
X_acq_time	= 3.49175808[s]
X_angle	= 45[deg]
X_atn	= 3.99[dB]
X_pulse	= 6.125[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 5[s]
Repetition_time	= 8.49175808[s]
Temp_get	= 22[dC]

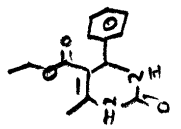

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Figure S7. ^{1}H NMR of **4**

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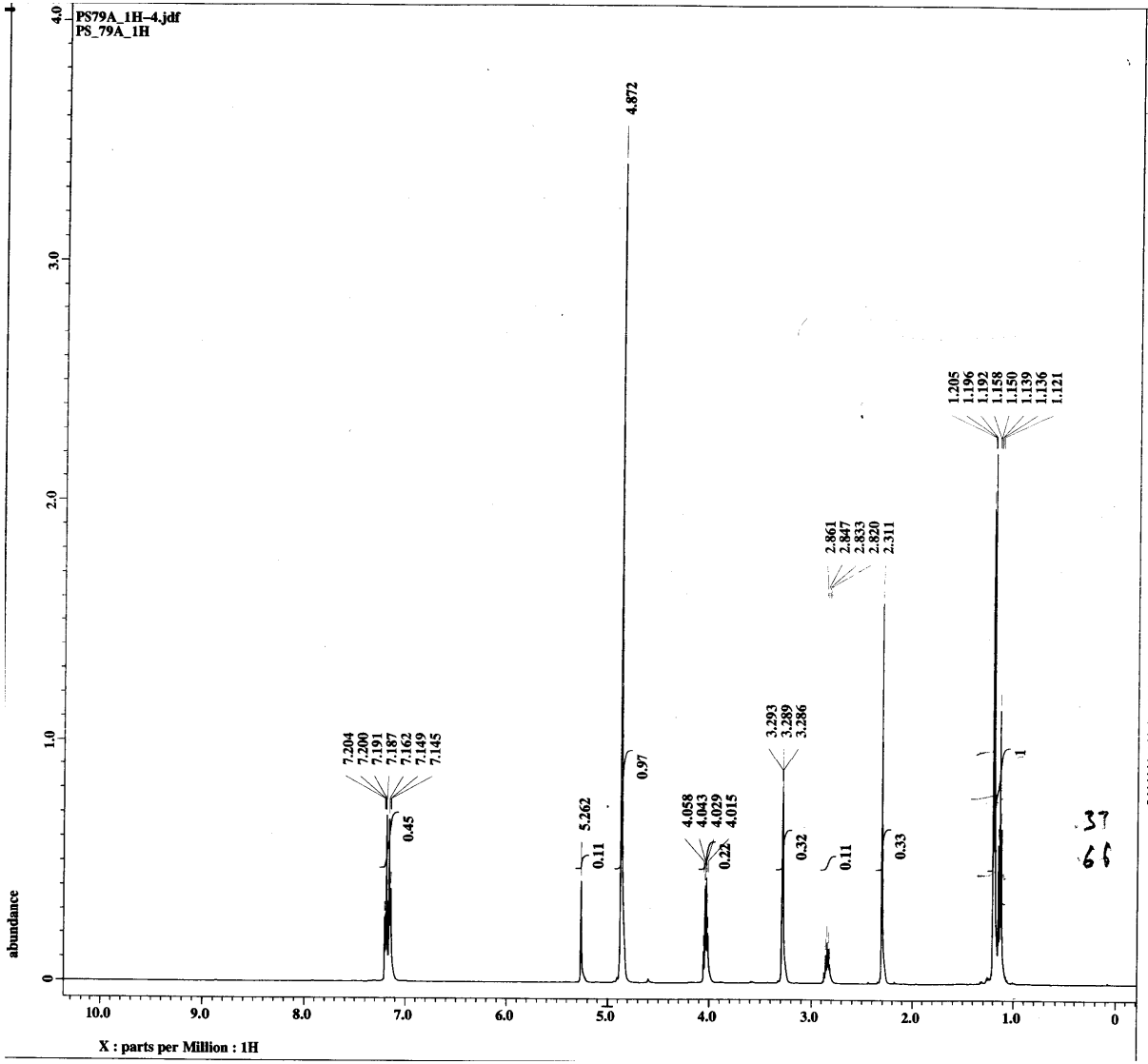

JEOL

Filename	= PS79A_1H-4.jdf
Author	= N.Ahmed
Experiment	= single_pulse.ex2
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Solvent	= METHANOL-D3
Creation_time	= 5-FEB-2008 12:32:05
Revision_time	= 5-FEB-2008 12:34:12
Current_time	= 5-FEB-2008 12:34:30
Comment	= PS_79A_1H
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 500
Spectrometer	= DELTA2_NMR
Field_strength	= 11.7473579[T] (500[MH
X_acq_duration	= 3.49175808[s]
X_domain	= 1H
X_freq	= 500.15991521[MHz]
X_offset	= 5.0[ppm]
X_points	= 32768
X_prescans	= 1
X_resolution	= 0.28638868[Hz]
X_sweep	= 9.38438438[kHz]
Irr_domain	= 1H
Irr_freq	= 500.15991521[MHz]
Irr_offset	= 5.0[ppm]
Tri_domain	= 1H
Tri_freq	= 500.15991521[MHz]
Tri_offset	= 5.0[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 12.25[us]
X_acq_time	= 3.49175808[s]
X_angle	= 45[deg]
X_atn	= 3.99[dB]
X_pulse	= 6.125[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 44
Relaxation_delay	= 5[s]
Repetition_time	= 8.49175808[s]
Temp_get	= 20.1[dC]

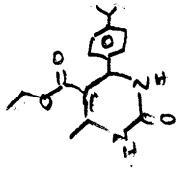
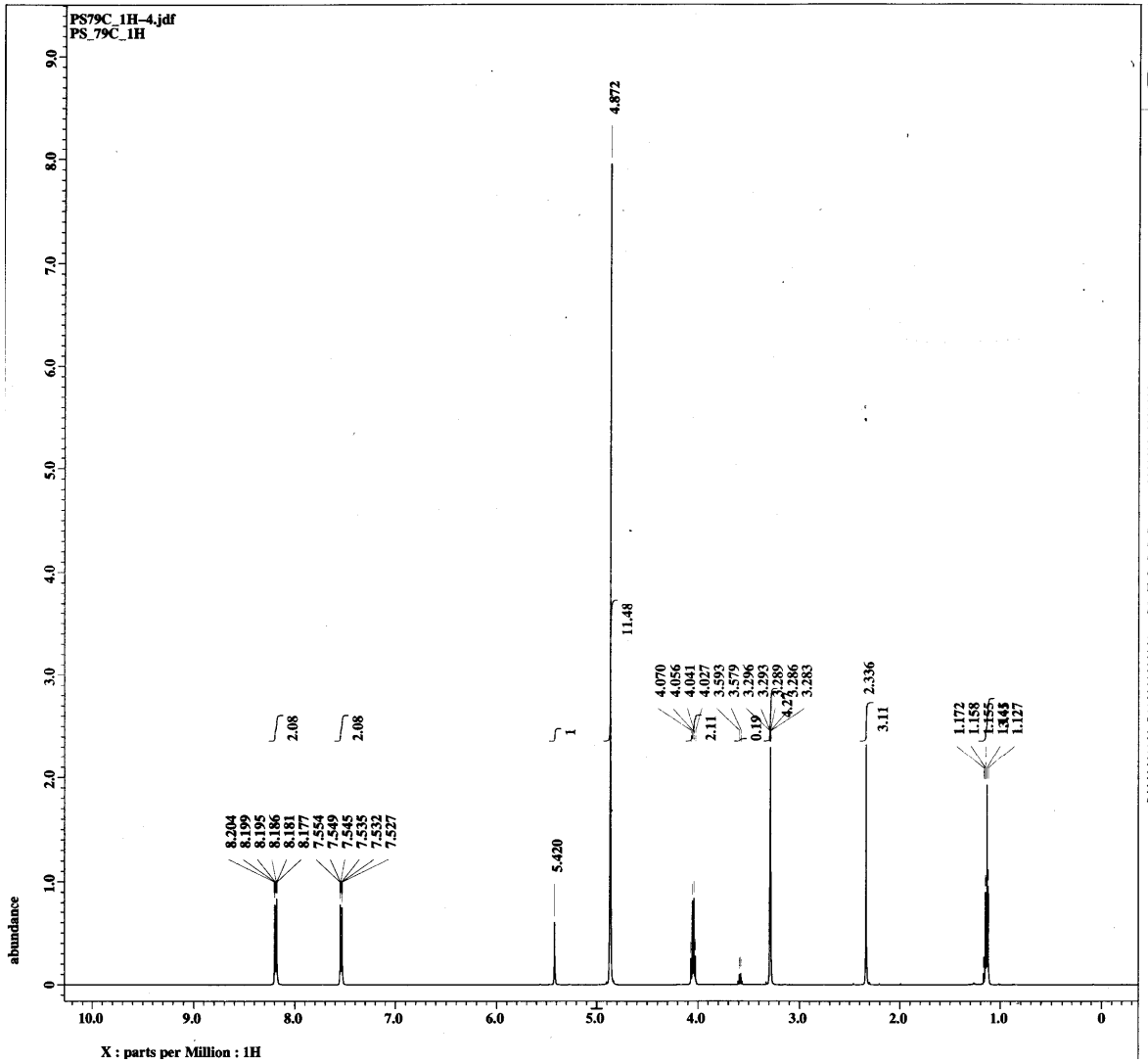


Figure S8. ^{1}H NMR of **5**



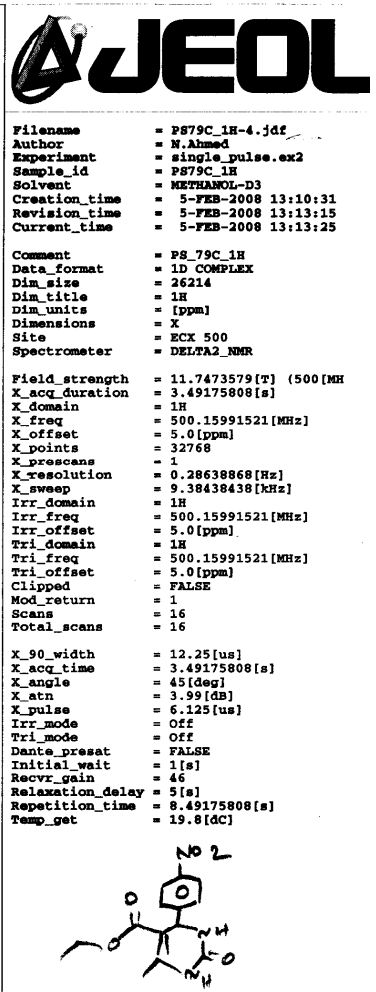


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Figure S9. Infrared spectrum of **2** recorded as a KBr pellet