SUPPORTING INFORMATION

Infrared multiple photon dissociation spectroscopy of a gas-phase oxo-molybdenum complex with 1,2-dithiolene ligands

Michael J. van Stipdonk[1*], Partha Basu[1*], Sara Dille[1], John K. Gibson[2], Giel Berden[3] and Jos Oomens[3,4]

[1]Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Ave, Pittsburgh PA 15282 USA
[2]Chemical Sciences Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720 USA
[3]Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Toernooiveld 7, 6525ED Nijmegen, The Netherlands
[4]van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands

Figure S1. CID spectra generated from solution of $MoO(mnt)_2^{2-}$: (a) CID (MS/MS stage) of m/z 524. (b) CID (MS^3 stage) of m/z 423 product derived from m/z 524 precursor.

Figure S2. CID spectra generated from solution of $MoO(mnt)_2^{2-}$: (a) CID (MS/MS stage) of m/z 197, (b) CID (MS^3 stage) of m/z 394 product derived from m/z 197 precursor.

Figure S3. Comparison of IRMPD and predicted spectra for cyano-coordinated Mo=O: (a) structure III and (b) structure IV.

Figure S4. Data for IRMPD of $[MoO(mnt_2]^{2-}$: (a) experimental IRMPD spectrum and (b) predicted spectrum for $[MoO(mnt_2]^{2-}$ in singlet spin state at M06-L/6-311+G(d) level of theory. IRMPD spectrum is included as grey trace in (b) to facilitate comparison.

Figure S5. Data for IRMPD of $[MoO(mnt_2]^{2-}$: (a) experimental IRMPD spectrum and (b) predicted spectrum for $[MoO(mnt_2]^{2-}$ in singlet spin state at B3LYP/6-311+G(3df) level of theory. IRMPD spectrum is included as grey trace in (b) to facilitate comparison.

Figure S6. Data for IRMPD of $[MoO(mnt_2]^{-}$: (a) experimental IRMPD spectrum, (b) predicted spectrum for $[MoO(mnt_2]^{-}$ in doublet spin state and (c) predicted spectrum for $[MoO(mnt_2]^{-}$ in quartet spin state. Predicted spectra are from calculations at the M06-L/6-311+G(d) level of theory. IRMPD spectrum is included as grey trace in (b) and (c) to facilitate comparison.

Figure S7. Data for IRMPD of $[MoO(mnt_2]^{-}$: (a) experimental IRMPD spectrum, (b) predicted spectrum for $[MoO(mnt_2]^{-}$ in doublet spin state and (c) predicted spectrum for $[MoO(mnt_2]^{-}$ in quartet spin state. Predicted spectra are from calculations at the B3LYP/6-311+G(3df) level of theory. IRMPD spectrum is included as grey trace in (b) and (c) to facilitate comparison.

Figure S8. General structure for $MoO(mnt)_2^{n-}$ with atom labels

Table S1. Dihedral angles predicted for $MoO(mnt)_2^{-}$ and $MoO(mnt)_2^{2-}$.

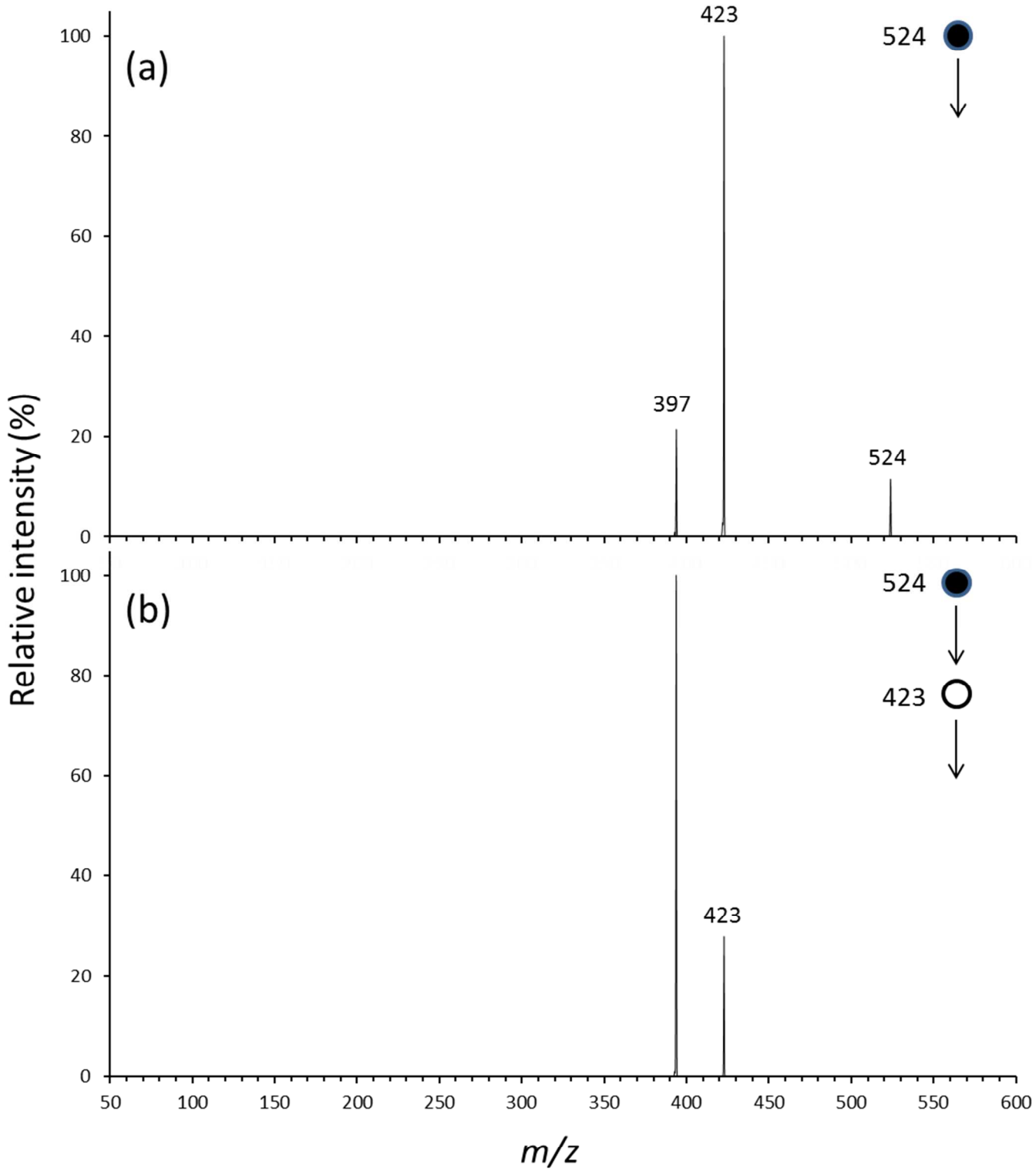
(a)
(b)
Relative intensity (%)
m/z
423
524
397
524
524
423
423
0
20
40
60
80
100
50
100
150
200
250
300
350
400
450
500
550
600

Figure S1.

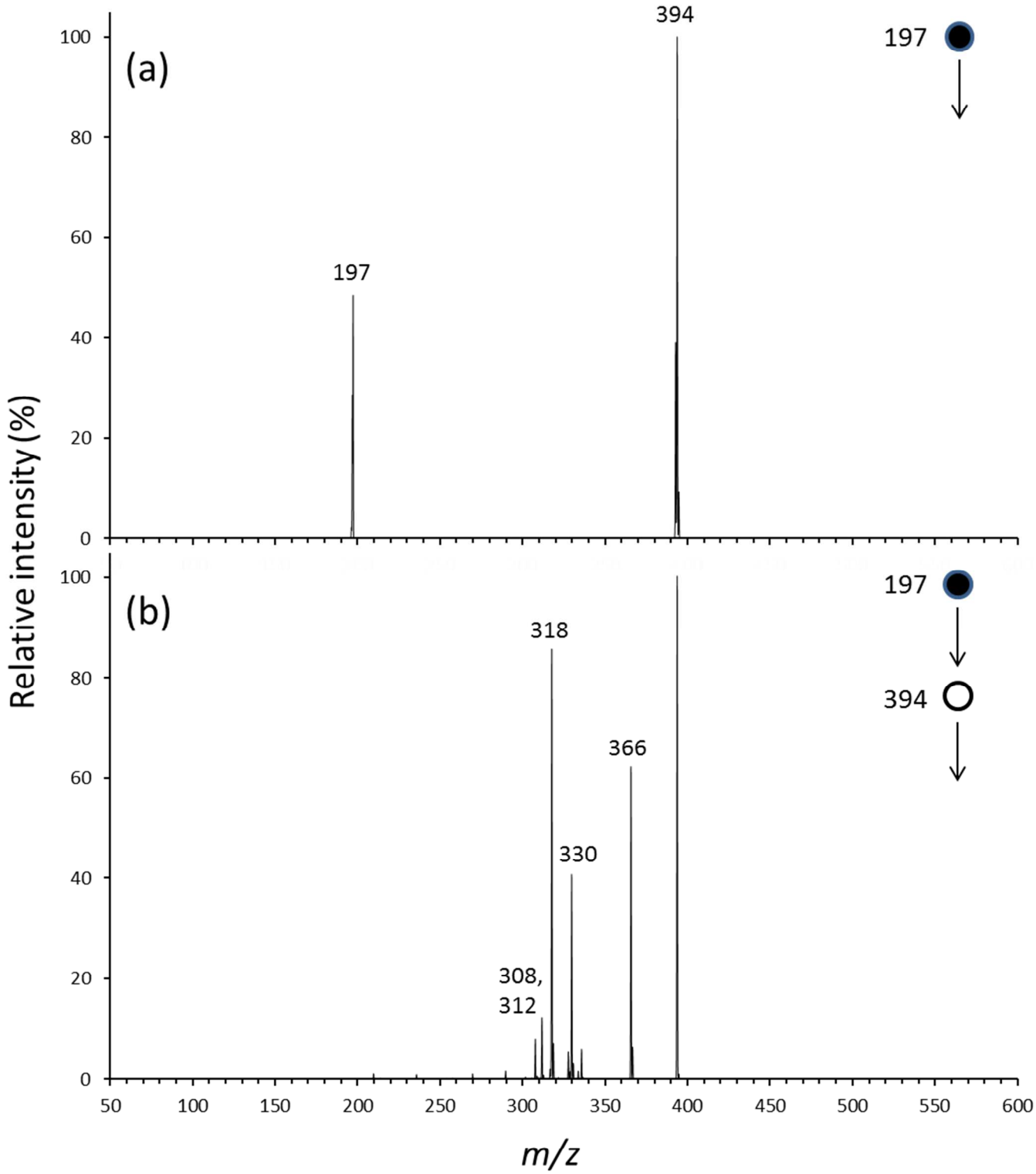
(a)
394
197
197
100
80
60
40
20
0
(b)
318
366
330
308,
312
394
197
Relative intensity (%)
50
100
150
200
250
300
350
400
450
500
550
600
m/z

Figure S2.

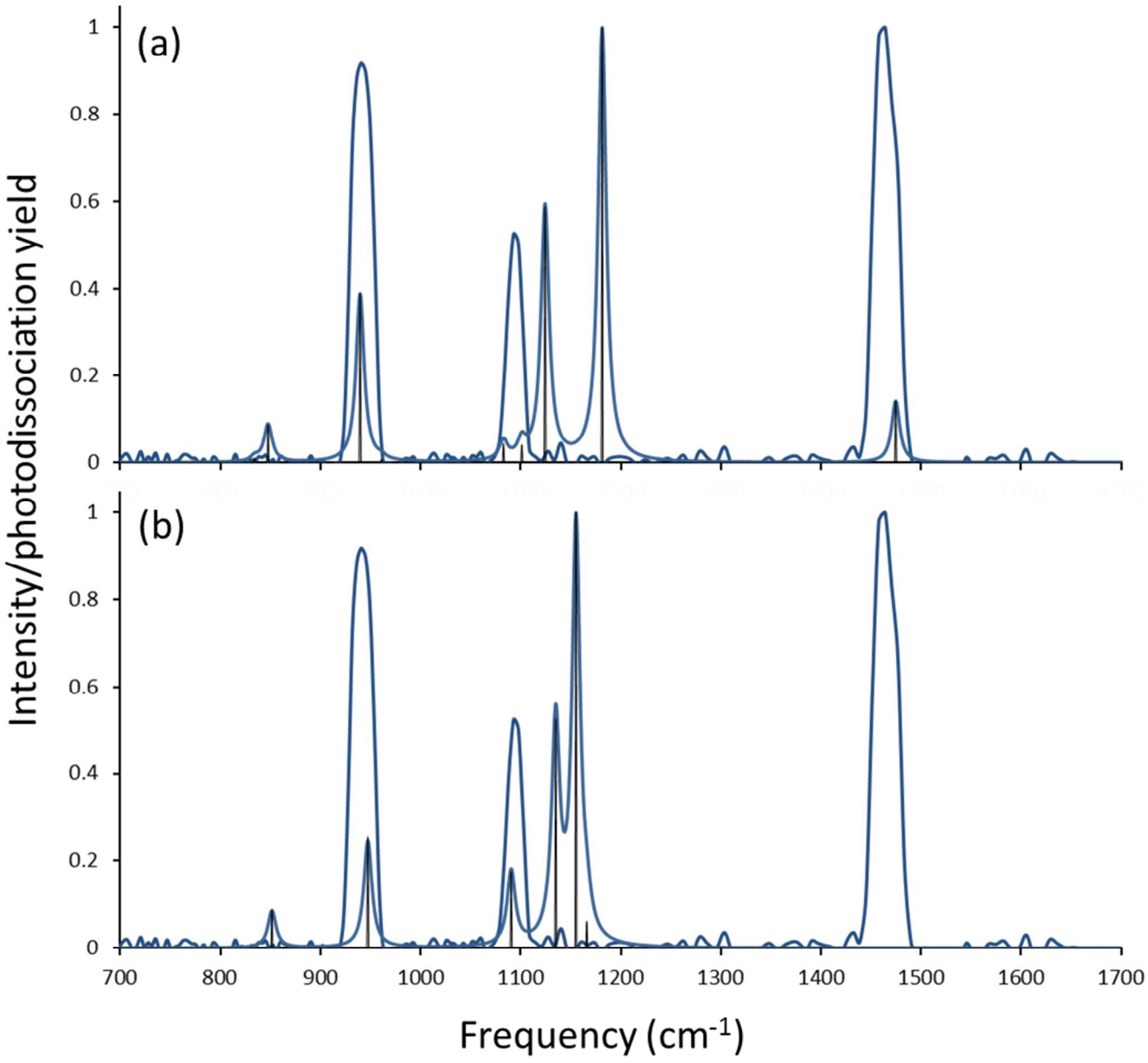
(a)
(b)
Intensity/photodissociation yield
Frequency (cm-1)
0
0.2
0.4
0.6
0.8
1
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700

Figure S3.

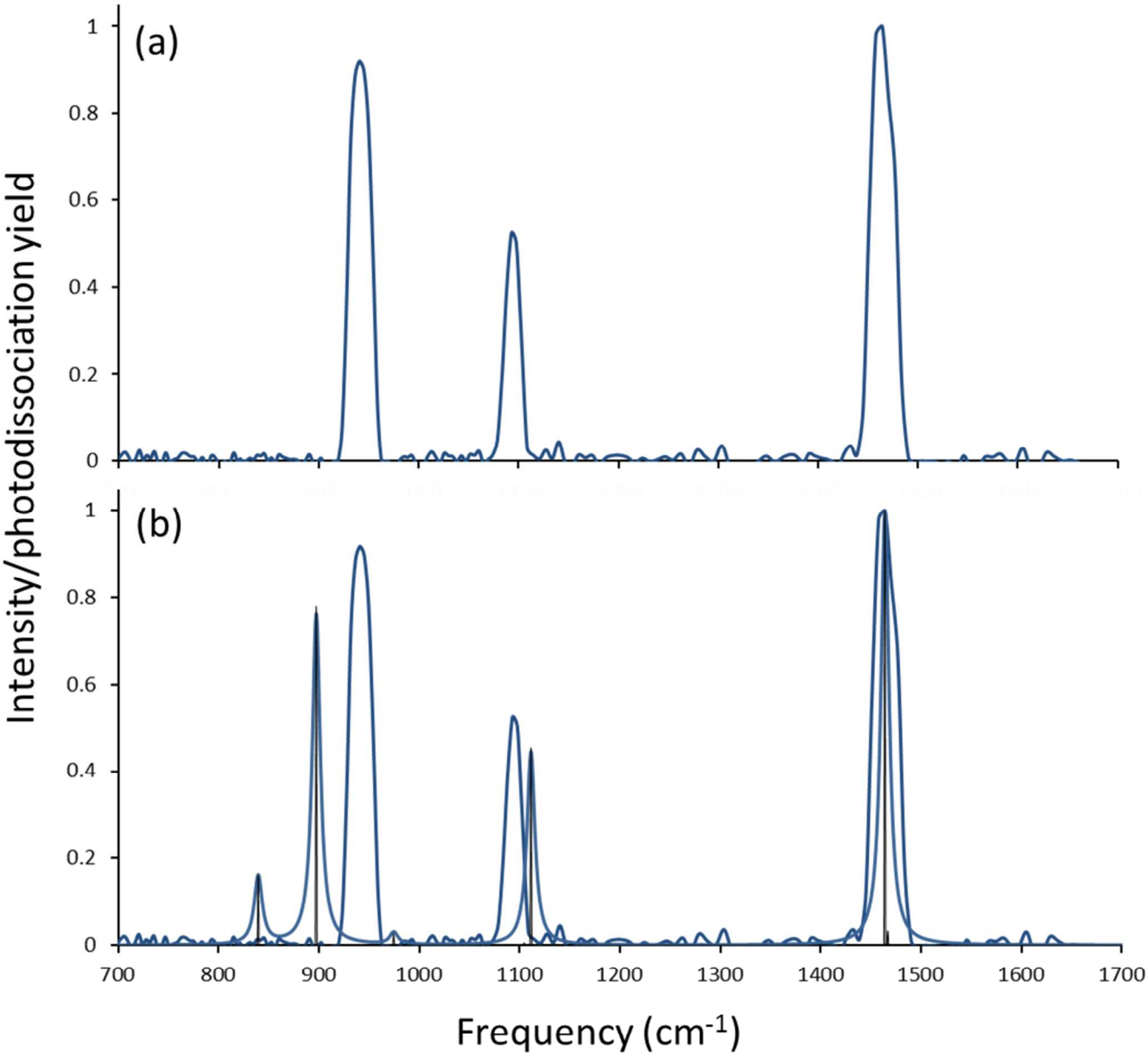
(a)
(b)
Intensity/photodissociation yield
Frequency (cm-1)
0
0.2
0.4
0.6
0.8
1
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700

Figure S4.

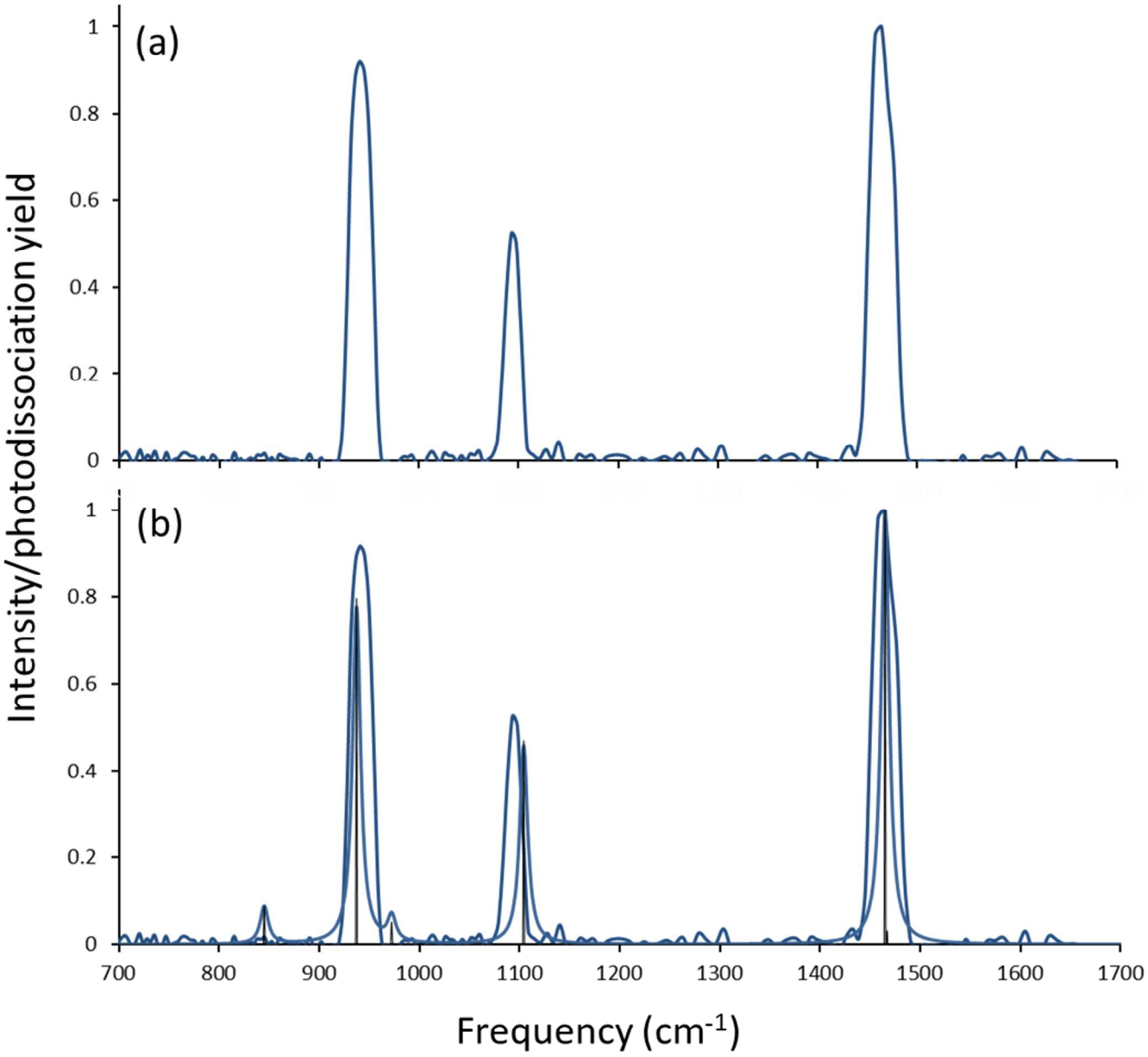
(a)
(b)
Intensity/photodissociation yield
Frequency (cm-1)
0
0.2
0.4
0.6
0.8
1
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700

Figure S5.

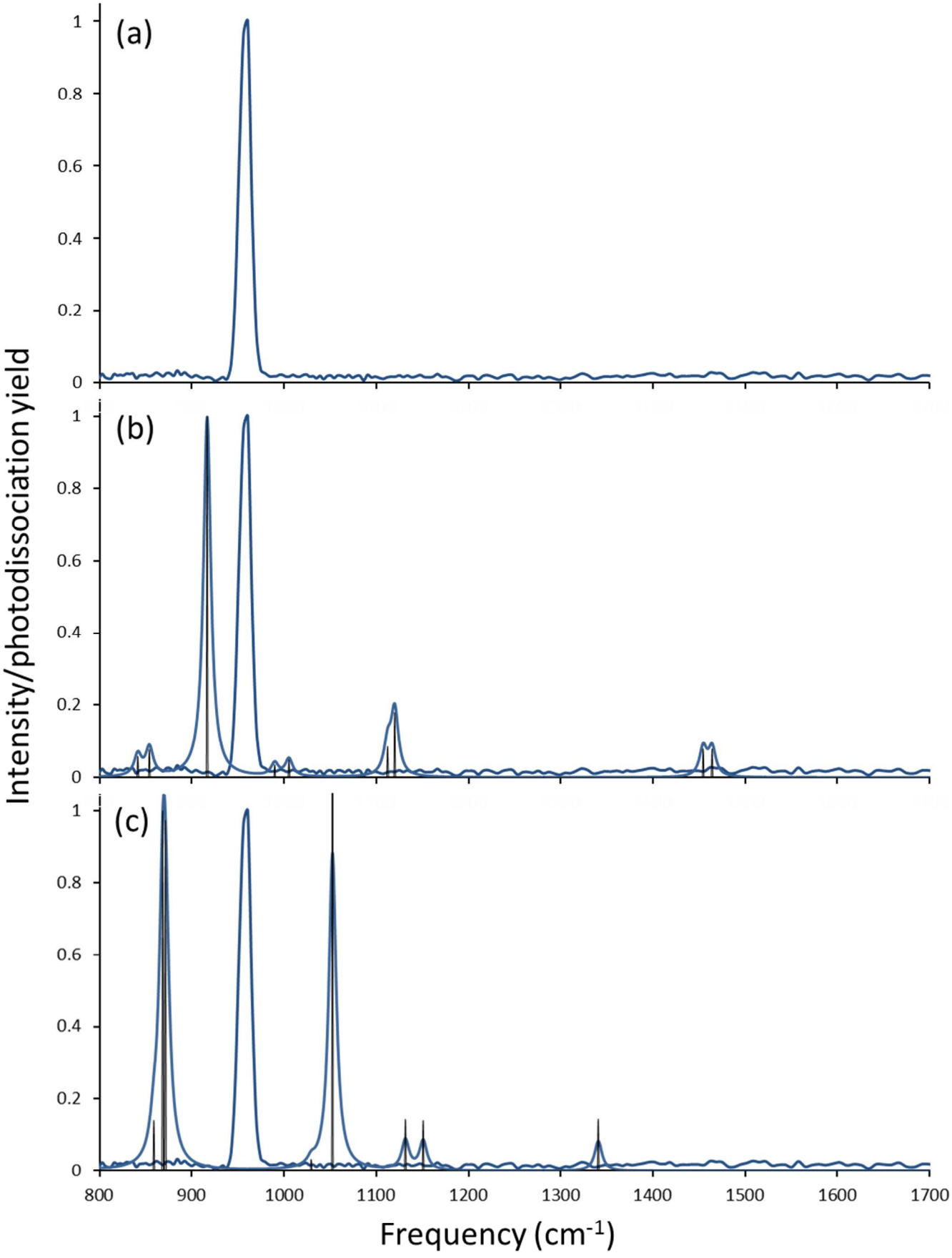
(a)
(b)
(c)
Intensity/photodissociation yield
Frequency (cm-1)
0
0.2
0.4
0.6
0.8
1
800
900
1000
1100
1200
1300
1400
1500
1600
1700

Figure S6.

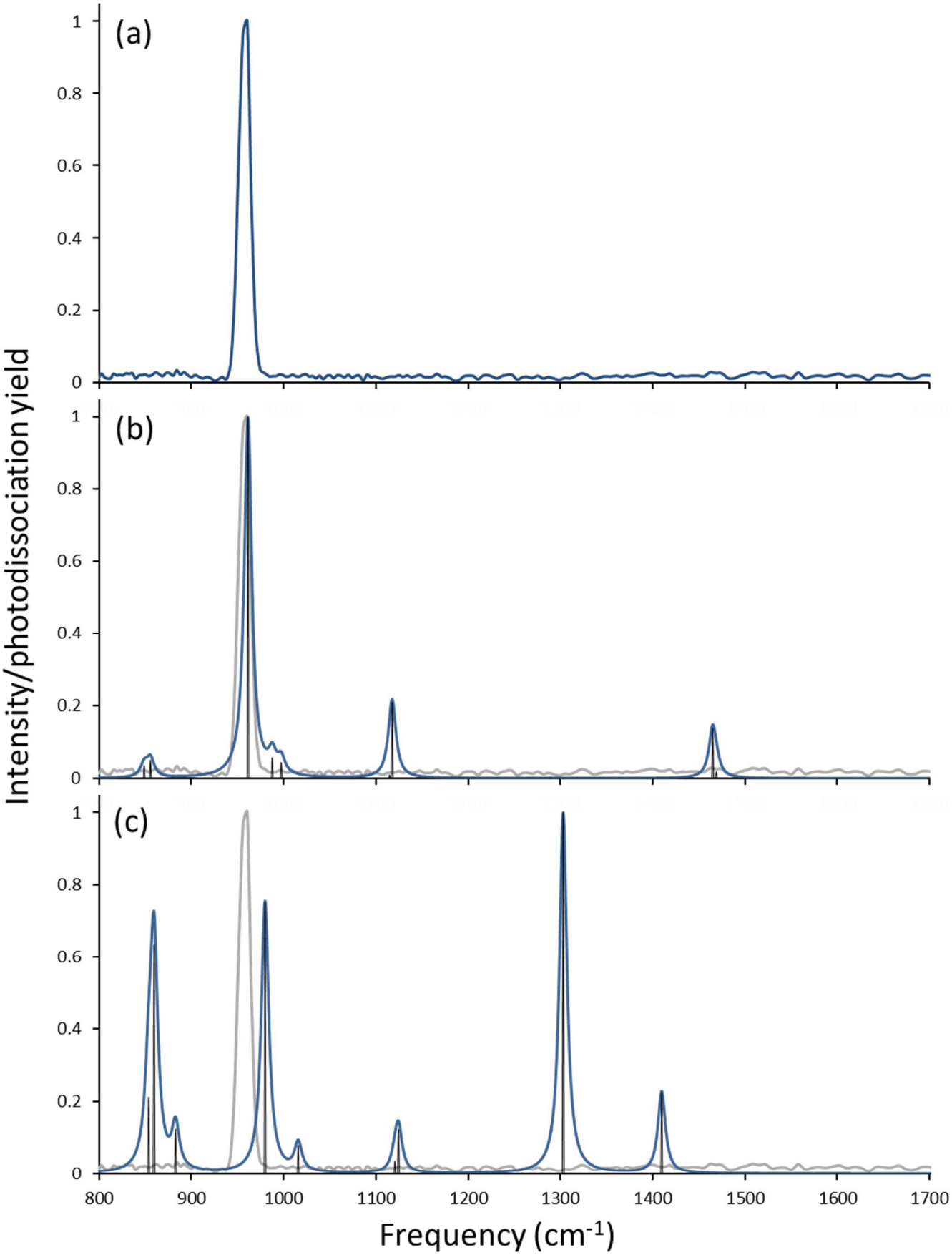
(a)
(b)
(c)
Intensity/photodissociation yield
Frequency (cm-1)
0
0.2
0.4
0.6
0.8
1
800
900
1000
1100
1200
1300
1400
1500
1600
1700

Figure S7.

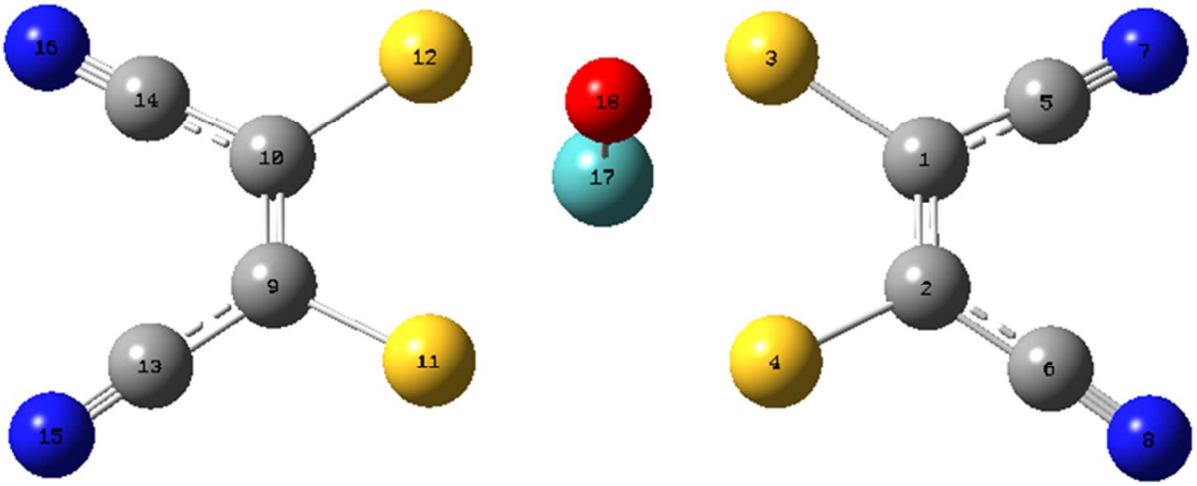

Figure S8.

Table S1.

$[MoO(mnt)_2]^{2-}$, singlet	**D18-17-12-10**	**D18-17-11-9**	**D18-17-3-1**	**D18-17-4-2**
B3LYP/6-31G(d)	-95.07	95.07	95.07	-95.07
B3LYP/6-311+G(d)	-95.42	95.42	95.41	-95.42
B3LYP/6-311+G(3df)	-95.55	95.55	95.53	-95.53
M06-L/6-311+G(d)	-95.67	95.68	95.68	-95.67

$[MoO(mnt)_2]^{-}$, doublet	**D18-17-12-10**	**D18-17-11-9**	**D18-17-3-1**	**D18-17-4-2**
B3LYP/6-31G(d)	-114.51	114.51	80.56	-80.56
B3LYP/6-311+G(d)	-115.00	115.00	81.23	-81.23
B3LYP/6-311+G(3df)	-114.38	114.37	81.75	-81.75
M06-L/6-311+G(d)	-114.85	114.85	79.25	-79.25

$[MoO(mnt)_2]^{-}$, quartet	**D18-17-12-10**	**D18-17-11-9**	**D18-17-3-1**	**D18-17-4-2**
B3LYP/6-31G(d)	-108.45	117.21	124.06	-75.58
B3LYP/6-311+G(d)	-108.61	117.94	125.03	-76.03
B3LYP/6-311+G(3df)	-109.02	116.51	123.92	-75.54
M06-L/6-311+G(d)	-108.82	120.19	133.65	-76.66