EXPERIMENTAL AND COMPUTATIONAL STUDIES ON THE EFFECT OF SECONDARY BONDING INTERACTIONS ON THE SPECTROSCOPIC PROPERTIES AND REACTIVITY OF ORGANO-CHALCOGEN COMPOUNDS

BY

PHILIP J. W. ELDER, B.SC.

A THESIS

SUBMITTED TO THE SCHOOL OF GRADUATE STUDIES

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS

FOR THE DEGREE

DOCTORATE OF PHILOSOPHY

SUPPLEMENTARY INFORMATION

MCMASTER UNIVERSITY

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S.1 Crystallographic Information File for ($C_{12}H_8N_2I_2$), **28**.

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_computing_publication_material 'Bruker SHELXTL'


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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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ZERR    4.00   0.0003   0.0012   0.0010   0.000   0.001   0.000
LATT  1
SYMM -X, 0.5+Y, 0.5-Z
SFAC C H N I
UNIT 48 32 8 8
TEMP 23.000

L.S. 4
BOND
```

```
FMAP 2
PLAN 2
WGHT    0.022000    0.959300
FVAR       0.09473
I1    4    0.379731    0.421269    0.585575    11.00000    0.07076    0.06947 =
       0.04103   -0.01095    0.01231   -0.01262
I2    4    1.123598    0.685129    0.927843    11.00000    0.07889    0.07057 =
       0.04760   -0.01477    0.01517   -0.02011
N1    3    0.815084    0.573629    0.783805    11.00000    0.04135    0.03942 =
       0.04190    0.00027    0.00559   -0.00540
C4    1    1.160784    0.673541    0.795004    11.00000    0.03743    0.03650 =
       0.04344   -0.00147    0.00625    0.00244
N2    3    0.680459    0.528087    0.733289    11.00000    0.03855    0.03895 =
       0.04215    0.00087    0.00381   -0.00487
C6    1    0.337255    0.428185    0.718500    11.00000    0.03767    0.03686 =
       0.03924    0.00285    0.00518    0.00325
C9    1    0.455864    0.484124    0.860210    11.00000    0.05292    0.05023 =
       0.03961   -0.00226    0.00261   -0.00998
C12   1    1.347208    0.721029    0.758544    11.00000    0.04227    0.03639 =
       0.06204    0.00134    0.00911   -0.00226
C13   1    1.214635    0.663015    0.619225    11.00000    0.05014    0.04880 =
       0.03775    0.00830    0.01413    0.00358
C14   1    0.492253    0.480545    0.772135    11.00000    0.03375    0.03746 =
       0.03824    0.00294    0.00456    0.00094
C15   1    0.118599    0.384032    0.839657    11.00000    0.05133    0.04798 =
       0.05591    0.01076    0.01615   -0.00490
C16   1    0.273400    0.435245    0.893173    11.00000    0.06050    0.05706 =
       0.03286    0.00453    0.00860   -0.00948
C17   1    1.003249    0.620454    0.743395    11.00000    0.03271    0.03238 =
       0.04289    0.00362    0.00416    0.00170
C18   1    1.032906    0.615232    0.654768    11.00000    0.04814    0.04136 =
       0.04285   -0.00154    0.00622   -0.00184
C20   1    1.373227    0.715171    0.671210    11.00000    0.04561    0.04453 =
       0.06676    0.01410    0.01955    0.00188
C1    1    0.149984    0.379745    0.752661    11.00000    0.04093    0.04012 =
       0.05375   -0.00056    0.00406   -0.00573
H3    2    0.045039    0.348697    0.715599    11.00000    0.04430
H4    2    1.229037    0.658219    0.564173    11.00000    0.04090
H5    2    1.493199    0.746155    0.643798    11.00000    0.05324
H6    2    0.558105    0.518537    0.894900    11.00000    0.04711
H7    2   -0.002132    0.349665    0.863329    11.00000    0.04474
H8    2    0.935374    0.580923    0.619524    11.00000    0.05207
H9    2    0.251689    0.438763    0.944238    11.00000    0.04889
H10   2    1.451254    0.753280    0.798753    11.00000    0.05331

HKLF 4

REM  diiodo_0m in P2(1)/c
REM R1 =  0.0271 for   2536 Fo > 4sig(Fo)  and  0.0397 for all   3186 data
REM    177 parameters refined using      0 restraints

END
```

```
WGHT      0.0207      0.9846
REM Highest difference peak  0.549,  deepest hole -0.559,  1-sigma level  0.073
Q1    1   1.2028  0.6453  0.9386  11.00000  0.05    0.55
Q2    1   0.3061  0.4613  0.5826  11.00000  0.05    0.52
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I2 I 1.12360(6) 0.685130(15) 0.927841(16) 0.06507(10) Uani 1 1 d . . .
N1 N 0.8151(5) 0.57361(14) 0.78379(17) 0.0409(6) Uani 1 1 d . . .
C4 C 1.1608(6) 0.67355(16) 0.7950(2) 0.0392(6) Uani 1 1 d . . .
N2 N 0.6805(5) 0.52811(14) 0.73327(16) 0.0400(5) Uani 1 1 d . . .
C6 C 0.3372(6) 0.42819(16) 0.71849(19) 0.0380(6) Uani 1 1 d . . .
C9 C 0.4562(7) 0.48417(18) 0.8602(2) 0.0480(8) Uani 1 1 d . . .
H9 H 0.5561 0.5197 0.8967 0.058 Uiso 1 1 calc R . .
C12 C 1.3472(7) 0.72094(17) 0.7587(2) 0.0470(7) Uani 1 1 d . . .
H12 H 1.4538 0.7564 0.7936 0.056 Uiso 1 1 calc R . .
C13 C 1.2147(7) 0.66291(18) 0.6191(2) 0.0448(7) Uani 1 1 d . . .
H13 H 1.2307 0.6599 0.5596 0.054 Uiso 1 1 calc R . .
C14 C 0.4922(6) 0.48053(16) 0.77214(19) 0.0366(6) Uani 1 1 d . . .
C15 C 0.1188(7) 0.38398(19) 0.8396(2) 0.0511(8) Uani 1 1 d . . .
H15 H -0.0076 0.3518 0.8624 0.061 Uiso 1 1 calc R . .
C16 C 0.2731(7) 0.43535(19) 0.8935(2) 0.0496(8) Uani 1 1 d . . .
H16 H 0.2537 0.4371 0.9528 0.059 Uiso 1 1 calc R . .
C17 C 1.0033(6) 0.62044(15) 0.7434(2) 0.0362(6) Uani 1 1 d . . .
C18 C 1.0329(7) 0.61520(17) 0.6547(2) 0.0441(7) Uani 1 1 d . . .
H18 H 0.9296 0.5794 0.6196 0.053 Uiso 1 1 calc R . .
C20 C 1.3732(7) 0.71516(18) 0.6711(2) 0.0510(8) Uani 1 1 d . . .
H20 H 1.4983 0.7467 0.6468 0.061 Uiso 1 1 calc R . .
C1 C 0.1496(6) 0.37975(17) 0.7525(2) 0.0452(7) Uani 1 1 d . . .
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I2 0.07885(19) 0.07055(18) 0.04757(14) -0.01476(11) 0.01515(12) -0.02010(13)
N1 0.0414(13) 0.0395(14) 0.0416(14) 0.0003(11) 0.0056(11) -0.0055(11)
C4 0.0373(15) 0.0367(16) 0.0436(16) -0.0016(12) 0.0063(12) 0.0024(12)
N2 0.0386(13) 0.0389(14) 0.0420(13) 0.0008(11) 0.0041(11) -0.0049(11)
C6 0.0377(15) 0.0368(16) 0.0394(15) 0.0028(12) 0.0052(12) 0.0032(12)
C9 0.0530(19) 0.0504(19) 0.0394(16) -0.0020(14) 0.0031(14) -0.0093(15)
C12 0.0422(17) 0.0358(17) 0.063(2) 0.0017(15) 0.0096(15) -0.0029(13)
C13 0.0494(18) 0.0482(18) 0.0389(16) 0.0088(14) 0.0138(14) 0.0035(14)
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C15 0.0510(19) 0.049(2) 0.056(2) 0.0108(16) 0.0161(16) -0.0045(15)
C16 0.059(2) 0.056(2) 0.0339(15) 0.0050(14) 0.0076(14) -0.0094(16)
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C18 0.0479(17) 0.0414(18) 0.0428(17) -0.0011(13) 0.0064(14) -0.0018(14)
C20 0.0454(18) 0.0444(19) 0.067(2) 0.0138(16) 0.0191(16) 0.0018(15)
C1 0.0412(16) 0.0397(17) 0.0541(19) -0.0001(14) 0.0049(14) -0.0053(13)

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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
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 and torsion angles; correlations between s.u.'s in cell parameters are only
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N1 C17 1.423(4) . ?
C4 C17 1.384(4) . ?
C4 C12 1.391(4) . ?
N2 C14 1.419(3) . ?
C6 C14 1.385(4) . ?
C6 C1 1.390(4) . ?
C9 C16 1.375(4) . ?
C9 C14 1.390(4) . ?
C9 H9 0.9300 . ?
C12 C20 1.374(5) . ?
C12 H12 0.9300 . ?
C13 C18 1.376(4) . ?
C13 C20 1.378(5) . ?
C13 H13 0.9300 . ?
C15 C1 1.370(4) . ?
C15 C16 1.374(5) . ?
C15 H15 0.9300 . ?
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C16 H16 0.9300 . ?
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N1 N2 C14 115.1(2) . . ?
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C20 C12 C4 119.7(3) . . ?
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C18 C13 C20 120.3(3) . . ?
C18 C13 H13 119.8 . . ?
C20 C13 H13 119.8 . . ?
C6 C14 C9 119.1(3) . . ?
C6 C14 N2 117.5(2) . . ?
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S.2 Crystallographic Information File for ($C_{14}H_{13}N_4O_2I$), **30**.

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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'I'  'I'  -0.4742   1.8119
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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N3 N 0.1966(6) 0.0000 0.1746(4) 0.0254(18) Uani 1 2 d S A 1
N1 N 0.1976(7) 0.0000 0.5516(5) 0.036(2) Uani 1 2 d S A 1
C4 C 0.2462(7) 0.0000 0.3091(5) 0.027(2) Uani 1 2 d S A 1
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N4 N 0.2669(8) 0.0000 -0.1440(5) 0.046(2) Uani 1 2 d S A 1
C12 C 0.1415(8) 0.0000 0.0340(6) 0.035(2) Uani 1 2 d S A 1
H12 H 0.0748 0.0000 0.0462 0.042 Uiso 1 2 calc SR A 1
C7 C 0.2205(8) 0.0000 0.0980(6) 0.032(2) Uani 1 2 d S A 1
C11 C 0.1529(8) 0.0000 -0.0456(5) 0.034(2) Uani 1 2 d S A 1
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C3 C 0.3261(7) 0.0000 0.3726(5) 0.027(2) Uani 1 2 d S A 1
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C14 C 0.1815(11) 0.0000 -0.2082(6) 0.062(4) Uani 1 2 d S A 1
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C4 0.032(6) 0.028(5) 0.020(5) 0.000 0.005(4) 0.000
N2 0.040(5) 0.024(4) 0.017(4) 0.000 0.006(4) 0.000
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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.
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N4 C14 1.446(14) . ?
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N4 C13 H13A 109.5 . . ?
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H13B C13 H13C 109.5 . . ?
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S.3 Crystallographic Information File for ($C_{32}H_{52}O_4N_4Te_4$), **64**.

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_publ_contact_author_address
;Department of Chemistry & Chemical Biology,
McMaster University
Hamilton, Ont., Canada
L8S 4M1
;
_publ_contact_author_email       vargas@chemistry.mcmaster.ca
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'K\"ubel, Joachim' "
'Elder, Philip J. W.' "
'Jenkins, Hilary A.' "
'Vargas-Baca, Ignacio' "

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_computing_cell_refinement       'Bruker SMART'
_computing_data_reduction        'Bruker SAINT'
_computing_structure_solution    'Bruker SHELXTL'
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_computing_molecular_graphics    'WINGX (Farrugia, 1999)'
_computing_publication_material  'WINGX (Farrugia, 1999)'

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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H4C H 0.5557 0.9969 0.3220 0.034 Uiso 1 1 calc R . .
C5 C 0.61783(17) 1.16527(15) 0.21108(12) 0.0211(4) Uani 1 1 d . . .
H5A H 0.6780 1.1818 0.1882 0.032 Uiso 1 1 calc R . .
H5B H 0.5958 1.2216 0.2361 0.032 Uiso 1 1 calc R . .
H5C H 0.5676 1.1472 0.1797 0.032 Uiso 1 1 calc R . .
C6 C 0.76515(14) 0.95286(15) 0.22680(10) 0.0166(3) Uani 1 1 d . . .
C7 C 0.79955(14) 0.87574(14) 0.18611(11) 0.0163(3) Uani 1 1 d . . .
C8 C 0.89636(15) 0.82858(17) 0.19294(12) 0.0222(4) Uani 1 1 d . . .
H8A H 0.8878 0.7582 0.1982 0.033 Uiso 1 1 calc R . .
H8B H 0.9297 0.8550 0.2309 0.033 Uiso 1 1 calc R . .
H8C H 0.9354 0.8414 0.1542 0.033 Uiso 1 1 calc R . .
H6A H 0.8080(19) 0.9726(19) 0.2587(14) 0.012(6) Uiso 1 1 d . . .

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O1 0.0165(6) 0.0213(7) 0.0221(8) -0.0073(6) -0.0077(6) 0.0030(5)
N1 0.0147(7) 0.0144(7) 0.0196(8) -0.0033(6) 0.0020(6) 0.0002(5)
C1 0.0165(8) 0.0136(7) 0.0140(8) -0.0006(6) -0.0007(7) -0.0022(6)
C2 0.0160(8) 0.0160(8) 0.0159(9) -0.0034(7) -0.0002(7) 0.0000(6)
C3 0.0252(10) 0.0245(10) 0.0246(11) -0.0111(9) -0.0046(9) 0.0022(8)
C4 0.0223(9) 0.0275(10) 0.0188(10) -0.0030(8) 0.0055(8) -0.0023(8)
C5 0.0250(10) 0.0146(8) 0.0236(11) -0.0015(8) 0.0014(8) 0.0004(7)
C6 0.0159(8) 0.0177(8) 0.0162(9) -0.0005(7) -0.0015(7) 0.0011(6)
C7 0.0148(8) 0.0160(8) 0.0182(9) 0.0005(7) 0.0000(7) 0.0007(6)
C8 0.0145(8) 0.0266(10) 0.0254(11) 0.0017(9) -0.0010(8) 0.0053(7)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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O1 N1 1.355(2) 12_766 ?
N1 C7 1.306(3) . ?
N1 O1 1.355(2) 15_565 ?
C1 C6 1.363(3) . ?
C1 C2 1.526(3) . ?
C2 C3 1.535(3) . ?
C2 C4 1.536(3) . ?
C2 C5 1.543(3) . ?
C3 H3A 0.9800 . ?
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C3 H3C 0.9800 . ?
C4 H4A 0.9800 . ?
C4 H4B 0.9800 . ?
C4 H4C 0.9800 . ?
C5 H5A 0.9800 . ?
C5 H5B 0.9800 . ?
C5 H5C 0.9800 . ?
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C6 C7 1.434(3) . ?
C6 H6A 0.93(3) . ?
C7 C8 1.487(3) . ?
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C8 H8B 0.9800 . ?
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Te1 Te1A 5.5382(7)

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C1 Te1 N1 77.88(7) . . ?
C1 Te1 O1 93.57(7) . . ?
N1 Te1 O1 171.45(6) . . ?
N1 O1 Te1 107.20(11) 12_766 . ?
C7 N1 O1 121.08(17) . 15_565 ?
C7 N1 Te1 115.43(14) . . ?
O1 N1 Te1 123.44(13) 15_565 . ?
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C3 C2 C4 107.60(19) . . ?
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C3 C2 C5 108.54(17) . . ?
C4 C2 C5 110.12(17) . . ?
C2 C3 H3A 109.5 . . ?
C2 C3 H3B 109.5 . . ?
H3A C3 H3B 109.5 . . ?
C2 C3 H3C 109.5 . . ?
H3A C3 H3C 109.5 . . ?
H3B C3 H3C 109.5 . . ?
C2 C4 H4A 109.5 . . ?
C2 C4 H4B 109.5 . . ?
H4A C4 H4B 109.5 . . ?
C2 C4 H4C 109.5 . . ?
H4A C4 H4C 109.5 . . ?
H4B C4 H4C 109.5 . . ?
C2 C5 H5A 109.5 . . ?
C2 C5 H5B 109.5 . . ?
H5A C5 H5B 109.5 . . ?
C2 C5 H5C 109.5 . . ?
H5A C5 H5C 109.5 . . ?
H5B C5 H5C 109.5 . . ?
C1 C6 C7 121.45(19) . . ?
C1 C6 H6A 123.4(17) . . ?
C7 C6 H6A 115.2(17) . . ?
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N1 C7 C6 114.02(18) . . ?
N1 C7 C8 121.78(19) . . ?
C6 C7 C8 124.16(19) . . ?
C7 C8 H8A 109.5 . . ?
C7 C8 H8B 109.5 . . ?
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S.4 Lowest 50 transitions for compounds **27**, **36**-**47**.

27

	E (eV)	λ (nm)	f
1	1.90	654	0.00001
2	2.17	570	0.54860
3	2.86	434	0.00002
4	2.96	419	0.52290
5	3.15	394	0.02042
6	3.26	380	0.00813
7	3.33	372	0.00000
8	3.55	349	0.10900
9	3.76	330	0.00007
10	3.89	319	0.01652
11	3.95	314	0.00000
12	3.97	312	0.00130
13	3.98	311	0.00000
14	4.04	307	0.00161
15	4.11	302	0.02981
16	4.22	294	0.08124
17	4.23	293	0.00000
18	4.44	279	0.00123
19	4.47	277	0.00935
20	4.65	267	0.00019
21	4.72	263	0.00005
22	4.80	258	0.00039
23	4.86	255	0.01408
24	4.87	255	0.00003
25	4.97	249	0.00049
26	5.04	246	0.00123
27	5.16	240	0.02647
28	5.20	238	0.01189
29	5.22	237	0.00206
30	5.25	236	0.00250
31	5.38	230	0.00000
32	5.42	229	0.00002
33	5.45	228	0.04864
34	5.54	224	0.02175
35	5.56	223	0.00001
36	5.60	221	0.00000
37	5.61	221	0.00016
38	5.63	220	0.00017
39	5.65	219	0.00619
40	5.67	219	0.00006
41	5.76	215	0.00012
42	5.79	214	0.00494
43	5.80	214	0.00000
44	5.83	213	0.00283
45	5.83	213	0.00000
46	5.87	211	0.00010
47	5.98	207	0.00093
48	6.00	207	0.00239
49	6.00	207	0.10830
50	6.04	205	0.07520

36

	E (eV)	λ (nm)	f
1	2.00	619	0.35190
2	2.58	481	0.04006
3	2.72	455	0.40960
4	2.80	443	0.00005
5	3.13	396	0.00195
6	3.25	382	0.00000
7	3.26	380	0.01540
8	3.60	344	0.12190
9	3.66	339	0.00003
10	3.68	337	0.00000
11	3.82	324	0.02568
12	3.85	322	0.03149
13	3.93	316	0.01848
14	4.06	305	0.02324
15	4.16	298	0.00818
16	4.17	297	0.00000
17	4.30	288	0.00296
18	4.32	287	0.00023
19	4.37	284	0.08652
20	4.51	275	0.00168
21	4.57	271	0.00023
22	4.62	268	0.06728
23	4.79	259	0.00010
24	4.83	257	0.01460
25	4.84	256	0.00004
26	4.84	256	0.02307
27	5.00	248	0.00008
28	5.00	248	0.12710
29	5.05	246	0.00002
30	5.16	240	0.13990
31	5.19	239	0.00711
32	5.19	239	0.00025
33	5.25	236	0.00000
34	5.27	235	0.00035
35	5.29	234	0.00317
36	5.32	233	0.00004
37	5.41	229	0.00571
38	5.44	228	0.00000
39	5.53	224	0.00118
40	5.54	224	0.00001
41	5.57	223	0.00912
42	5.61	221	0.01699
43	5.61	221	0.00006
44	5.63	220	0.00003
45	5.65	220	0.00000
46	5.69	218	0.00024
47	5.71	217	0.00016
48	5.71	217	0.10460
49	5.74	216	0.02503
50	5.76	215	0.00129

37

E (eV)	λ (nm)	f
1.96	632	0.27020
2.04	607	0.00000
2.30	539	0.15250
2.48	500	0.00000
2.68	463	0.36480
2.85	434	0.00787
2.92	425	0.00002
3.09	401	0.03756
3.15	394	0.00509
3.19	388	0.00000
3.37	368	0.00003
3.52	352	0.04729
3.60	345	0.00002
3.69	336	0.04041
3.82	325	0.06885
3.91	317	0.03213
4.03	308	0.00948
4.06	305	0.00002
4.15	299	0.00067
4.15	299	0.00000
4.22	294	0.03500
4.23	293	0.03000
4.27	290	0.00000
4.29	289	0.00002
4.33	286	0.00203
4.37	284	0.00015
4.50	275	0.04537
4.54	273	0.00002
4.54	273	0.00024
4.54	273	0.00571
4.74	262	0.00000
4.76	261	0.03258
4.78	259	0.07506
4.83	257	0.00004
4.85	255	0.01288
4.89	254	0.00099
4.94	251	0.00006
4.97	249	0.02796
5.08	244	0.00000
5.11	243	0.01886
5.20	239	0.11410
5.21	238	0.00000
5.23	237	0.00316
5.27	235	0.00122
5.28	235	0.00023
5.28	235	0.00588
5.34	232	0.00036
5.35	232	0.04724
5.37	231	0.00294
5.40	230	0.00000

	38			39		
	E (eV)	λ (nm)	f	E (eV)	λ (nm)	f
1	1.67	741	0.00001	1.27	977	0.00001
2	1.74	714	0.07509	1.35	918	0.02664
3	2.01	616	0.00000	1.65	753	0.00000
4	2.13	583	0.31380	2.05	606	0.18990
5	2.54	489	0.26740	2.15	577	0.00000
6	2.55	486	0.00001	2.23	555	0.30490
7	2.72	456	0.00581	2.52	492	0.00008
8	2.90	428	0.00005	2.65	468	0.01003
9	2.90	428	0.17060	2.83	438	0.30670
10	3.15	393	0.00314	3.16	393	0.00360
11	3.20	388	0.00000	3.22	385	0.00000
12	3.40	364	0.01168	3.31	374	0.00923
13	3.60	345	0.00002	3.33	373	0.00000
14	3.61	343	0.03741	3.34	371	0.01892
15	3.67	337	0.07223	3.39	366	0.00037
16	3.72	334	0.00001	3.48	356	0.00170
17	3.83	324	0.07465	3.50	354	0.00000
18	3.91	317	0.00000	3.54	350	0.01701
19	3.94	315	0.00017	3.62	337	0.00002
20	3.97	312	0.00379	3.62	336	0.12370
21	4.05	306	0.00277	3.68	333	0.00008
22	4.06	305	0.00002	3.68	327	0.00005
23	4.15	299	0.01424	3.86	324	0.00008
24	4.16	298	0.00000	3.91	316	0.01075
25	4.17	297	0.01833	3.97	312	0.01098
26	4.22	294	0.00584	4.10	308	0.01228
27	4.25	292	0.00001	4.15	303	0.00006
28	4.26	291	0.00001	4.15	300	0.01731
29	4.31	288	0.00121	4.18	298	0.00003
30	4.34	286	0.01101	4.19	296	0.03499
31	4.39	282	0.02457	4.20	295	0.00000
32	4.50	276	0.03619	4.22	290	0.02487
33	4.55	273	0.00026	4.30	289	0.00171
34	4.56	272	0.00061	4.47	287	0.04340
35	4.59	270	0.00001	4.50	286	0.00005
36	4.61	269	0.07981	4.53	285	0.09510
37	4.80	259	0.00319	4.54	280	0.00118
38	4.80	258	0.00527	4.56	277	0.00000
39	4.83	257	0.00613	4.56	276	0.00037
40	4.93	252	0.00008	4.57	274	0.05689
41	4.99	249	0.00004	4.60	273	0.00731
42	5.00	248	0.00149	4.66	272	0.00000
43	5.03	246	0.00002	4.73	267	0.28760
44	5.03	246	0.02890	4.78	266	0.00004
45	5.04	246	0.00000	4.93	265	0.06679
46	5.05	246	0.10010	4.95	261	0.00075
47	5.12	242	0.00723	4.96	256	0.01403
48	5.20	238	0.00017	5.00	254	0.00000
49	5.21	238	0.00000	5.01	253	0.00019
50	5.21	238	0.11340	5.04	250	0.12530

	40			41		
	E (eV)	λ (nm)	f	E (eV)	λ (nm)	f
1	1.96	634	0.28290	1.88	659	0.19670
2	2.43	511	0.13130	2.27	547	0.00000
3	2.68	463	0.38300	2.28	545	0.21600
4	2.81	441	0.00002	2.62	473	0.00000
5	3.13	396	0.01697	2.63	472	0.36890
6	3.15	393	0.01451	2.90	428	0.00062
7	3.22	385	0.00000	3.04	408	0.06615
8	3.56	348	0.09918	3.15	393	0.00377
9	3.62	343	0.00001	3.16	392	0.00003
10	3.63	342	0.00777	3.20	387	0.00000
11	3.72	333	0.00002	3.53	352	0.00004
12	3.82	325	0.05882	3.53	351	0.06112
13	3.91	317	0.04800	3.59	345	0.00002
14	4.04	307	0.00967	3.73	332	0.01126
15	4.15	299	0.00047	3.75	330	0.05649
16	4.17	298	0.00009	3.87	321	0.06179
17	4.17	297	0.00014	3.98	311	0.00009
18	4.25	292	0.06817	4.02	309	0.01254
19	4.26	291	0.01098	4.02	308	0.00119
20	4.41	281	0.01830	4.15	299	0.00319
21	4.52	274	0.03662	4.17	298	0.00000
22	4.55	272	0.00026	4.20	295	0.05564
23	4.70	264	0.08791	4.24	292	0.00521
24	4.71	263	0.00148	4.25	292	0.00013
25	4.78	259	0.00104	4.29	289	0.00002
26	4.79	259	0.01099	4.41	281	0.06801
27	4.80	258	0.10000	4.49	276	0.00000
28	4.81	258	0.00001	4.50	276	0.01119
29	4.94	251	0.00001	4.50	276	0.00108
30	5.01	248	0.00001	4.55	273	0.00035
31	5.02	247	0.03626	4.68	265	0.10260
32	5.06	245	0.00013	4.70	264	0.00000
33	5.15	241	0.00166	4.77	260	0.01068
34	5.19	239	0.00023	4.79	259	0.00020
35	5.23	237	0.00000	4.86	255	0.01193
36	5.25	236	0.06438	4.88	254	0.00447
37	5.25	236	0.00010	4.89	254	0.00001
38	5.31	233	0.00347	4.91	252	0.00000
39	5.32	233	0.00100	4.93	252	0.00318
40	5.36	231	0.00123	5.12	242	0.07647
41	5.37	231	0.02300	5.14	241	0.00034
42	5.43	229	0.00001	5.16	240	0.00005
43	5.49	226	0.00016	5.17	240	0.02763
44	5.51	225	0.00262	5.18	239	0.00028
45	5.57	223	0.00000	5.22	237	0.00000
46	5.59	222	0.02348	5.23	237	0.00443
47	5.61	221	0.00000	5.25	236	0.00059
48	5.64	220	0.01956	5.30	234	0.08213
49	5.64	220	0.00290	5.31	234	0.01038
50	5.67	219	0.00004	5.34	232	0.00093

	42			43		
	E (eV)	λ (nm)	f	E (eV)	λ (nm)	f
1	1.73	717	0.09600	1.40	885	0.03605
2	1.93	642	0.00000	1.47	845	0.00001
3	2.16	575	0.27120	1.86	666	0.00000
4	2.22	560	0.00000	2.05	606	0.19110
5	2.53	491	0.32720	2.28	545	0.31410
6	2.68	463	0.00798	2.36	526	0.00000
7	2.83	439	0.00001	2.56	484	0.02765
8	2.94	422	0.14620	2.75	451	0.00009
9	3.11	398	0.00007	2.84	436	0.28020
10	3.16	393	0.00303	3.16	393	0.00309
11	3.21	387	0.00000	3.23	384	0.00000
12	3.40	364	0.00931	3.28	378	0.00598
13	3.58	347	0.04065	3.28	378	0.00068
14	3.60	345	0.00002	3.37	368	0.02655
15	3.64	340	0.05791	3.50	355	0.00131
16	3.69	336	0.00031	3.55	350	0.00000
17	3.80	326	0.07734	3.59	345	0.04986
18	3.95	314	0.02209	3.60	345	0.00032
19	3.99	311	0.00000	3.61	343	0.00000
20	4.00	310	0.00644	3.63	342	0.09638
21	4.07	304	0.00050	3.71	334	0.00000
22	4.11	301	0.00103	3.90	318	0.02683
23	4.13	300	0.02080	3.90	318	0.00002
24	4.17	298	0.03063	3.94	314	0.00010
25	4.17	297	0.00002	3.95	314	0.00152
26	4.18	297	0.00001	3.99	311	0.00419
27	4.18	296	0.00496	4.07	305	0.00009
28	4.25	291	0.00237	4.11	301	0.00986
29	4.27	291	0.00001	4.15	299	0.01510
30	4.39	282	0.03366	4.19	296	0.00000
31	4.45	279	0.00003	4.23	293	0.06613
32	4.47	277	0.03585	4.28	290	0.00385
33	4.54	273	0.01984	4.34	286	0.00005
34	4.55	273	0.00029	4.40	282	0.00001
35	4.59	270	0.07362	4.42	281	0.04333
36	4.71	264	0.00002	4.49	276	0.07739
37	4.72	263	0.00763	4.51	275	0.00178
38	4.77	260	0.00269	4.55	272	0.00031
39	4.80	258	0.00019	4.58	271	0.16820
40	4.85	255	0.00388	4.66	266	0.00008
41	4.86	255	0.00000	4.70	264	0.01967
42	4.90	253	0.00000	4.73	262	0.06370
43	5.04	246	0.00016	4.77	260	0.00006
44	5.05	246	0.15270	4.79	259	0.10170
45	5.09	244	0.00000	4.84	256	0.00181
46	5.11	243	0.00865	4.87	255	0.00009
47	5.14	241	0.00018	4.90	253	0.00002
48	5.14	241	0.09953	4.92	252	0.00007
49	5.15	241	0.13470	4.94	251	0.01227
50	5.23	237	0.00000	4.96	250	0.09563

	44			45		
	E (eV)	λ (nm)	f	E (eV)	λ (nm)	f
1	1.79	693	0.14370	1.73	718	0.12130
2	2.29	542	0.24930	2.22	557	0.24820
3	2.54	489	0.32850	2.37	524	0.00003
4	2.73	454	0.00009	2.49	498	0.35610
5	3.00	413	0.05241	2.81	442	0.00000
6	3.15	394	0.00258	2.96	418	0.07001
7	3.22	385	0.00000	3.01	411	0.00507
8	3.47	357	0.01521	3.14	395	0.00279
9	3.54	350	0.05004	3.21	386	0.00000
10	3.58	346	0.00001	3.27	379	0.00000
11	3.64	341	0.10490	3.51	353	0.03795
12	3.65	339	0.00000	3.59	346	0.00000
13	3.79	327	0.11010	3.59	345	0.09370
14	3.97	313	0.00057	3.70	336	0.03774
15	4.00	310	0.00798	3.71	334	0.00004
16	4.12	301	0.00546	3.79	327	0.09006
17	4.17	297	0.00000	3.85	322	0.00019
18	4.17	297	0.05112	3.88	320	0.00396
19	4.23	293	0.01399	3.99	311	0.00598
20	4.28	289	0.04679	4.02	309	0.00038
21	4.28	289	0.00025	4.12	301	0.00887
22	4.39	283	0.02671	4.17	298	0.04308
23	4.45	279	0.05823	4.18	297	0.00001
24	4.51	275	0.00048	4.22	294	0.04018
25	4.59	270	0.00642	4.26	291	0.00555
26	4.63	268	0.10480	4.28	290	0.00073
27	4.72	262	0.00002	4.38	283	0.00005
28	4.76	260	0.00019	4.43	280	0.07384
29	4.77	260	0.00508	4.51	275	0.00004
30	4.83	257	0.00001	4.52	275	0.05258
31	4.85	256	0.00086	4.53	274	0.00027
32	4.85	255	0.00018	4.54	273	0.00017
33	4.90	253	0.00016	4.58	271	0.00314
34	4.98	249	0.00002	4.65	266	0.01939
35	5.06	245	0.00303	4.73	262	0.00572
36	5.11	243	0.01743	4.81	258	0.00237
37	5.23	237	0.00033	4.86	255	0.00000
38	5.23	237	0.00007	4.89	254	0.00000
39	5.23	237	0.00320	4.93	252	0.00013
40	5.25	236	0.00429	4.99	248	0.00867
41	5.28	235	0.01650	5.01	247	0.00470
42	5.31	233	0.04910	5.04	246	0.00016
43	5.36	231	0.00006	5.07	245	0.06494
44	5.38	231	0.00238	5.12	242	0.07807
45	5.40	230	0.00001	5.18	239	0.00361
46	5.44	228	0.00091	5.23	237	0.00107
47	5.45	228	0.00910	5.23	237	0.00000
48	5.53	224	0.02703	5.26	236	0.00001
49	5.58	222	0.00005	5.27	235	0.03676
50	5.61	221	0.00218	5.27	235	0.02411

	46			47		
	E (eV)	λ (nm)	f	E (eV)	λ (nm)	f
1	1.65	753	0.09341	1.42	873	0.05118
2	2.10	589	0.00001	1.61	771	0.00000
3	2.16	575	0.22530	1.98	625	0.00000
4	2.36	526	0.00001	2.01	618	0.13790
5	2.43	510	0.37410	2.28	545	0.37200
6	2.67	464	0.00526	2.45	507	0.05601
7	2.93	424	0.10330	2.50	496	0.00000
8	3.00	413	0.00000	2.82	440	0.18540
9	3.14	395	0.00259	2.88	431	0.00005
10	3.22	385	0.00000	3.13	396	0.00162
11	3.26	380	0.00004	3.17	391	0.00624
12	3.43	362	0.00688	3.23	383	0.00000
13	3.52	353	0.01237	3.30	375	0.00123
14	3.54	350	0.08314	3.34	371	0.04305
15	3.58	347	0.00001	3.45	359	0.00380
16	3.61	343	0.00056	3.56	348	0.12300
17	3.64	341	0.05435	3.56	348	0.00002
18	3.75	331	0.10750	3.66	339	0.05681
19	3.87	320	0.00018	3.68	337	0.00049
20	3.98	311	0.00520	3.69	336	0.00004
21	4.01	309	0.00126	3.72	333	0.00024
22	4.09	303	0.01808	3.80	327	0.02733
23	4.14	299	0.00870	3.82	324	0.00002
24	4.15	299	0.00005	3.93	316	0.00026
25	4.15	298	0.02304	3.97	312	0.00298
26	4.18	297	0.00001	4.03	308	0.00003
27	4.26	291	0.00280	4.10	303	0.01082
28	4.30	288	0.00001	4.13	300	0.00685
29	4.38	283	0.00008	4.16	298	0.00004
30	4.39	283	0.10870	4.19	296	0.00001
31	4.42	281	0.00001	4.21	295	0.06707
32	4.45	278	0.01298	4.27	290	0.00272
33	4.52	274	0.00122	4.29	289	0.00014
34	4.53	274	0.00090	4.32	287	0.07155
35	4.54	273	0.04684	4.33	286	0.00007
36	4.57	271	0.00001	4.36	285	0.00001
37	4.57	271	0.00108	4.42	280	0.00923
38	4.63	268	0.02664	4.47	277	0.10760
39	4.69	265	0.00570	4.50	276	0.00039
40	4.77	260	0.01045	4.53	274	0.00501
41	4.79	259	0.00029	4.55	273	0.00005
42	4.86	255	0.00003	4.56	272	0.05593
43	4.86	255	0.00069	4.65	267	0.00375
44	4.93	251	0.00553	4.66	266	0.00000
45	4.96	250	0.06606	4.67	265	0.09392
46	4.98	249	0.13580	4.76	261	0.00281
47	5.02	247	0.00015	4.85	256	0.00002
48	5.08	244	0.02262	4.89	254	0.09295
49	5.12	242	0.00506	4.89	253	0.00021
50	5.22	237	0.03151	4.96	250	0.01271