

# CHEMISTRY

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### Supporting Information

#### **Mercury(II) Binding to Metallothionein in *Mytilus edulis* revealed by High Energy-Resolution XANES Spectroscopy**

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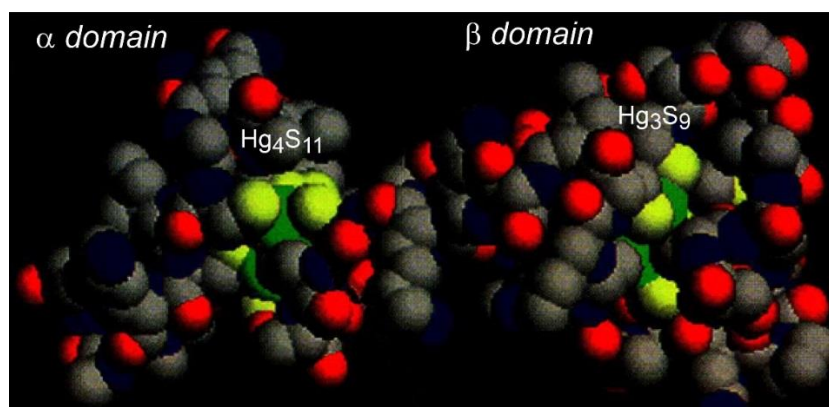
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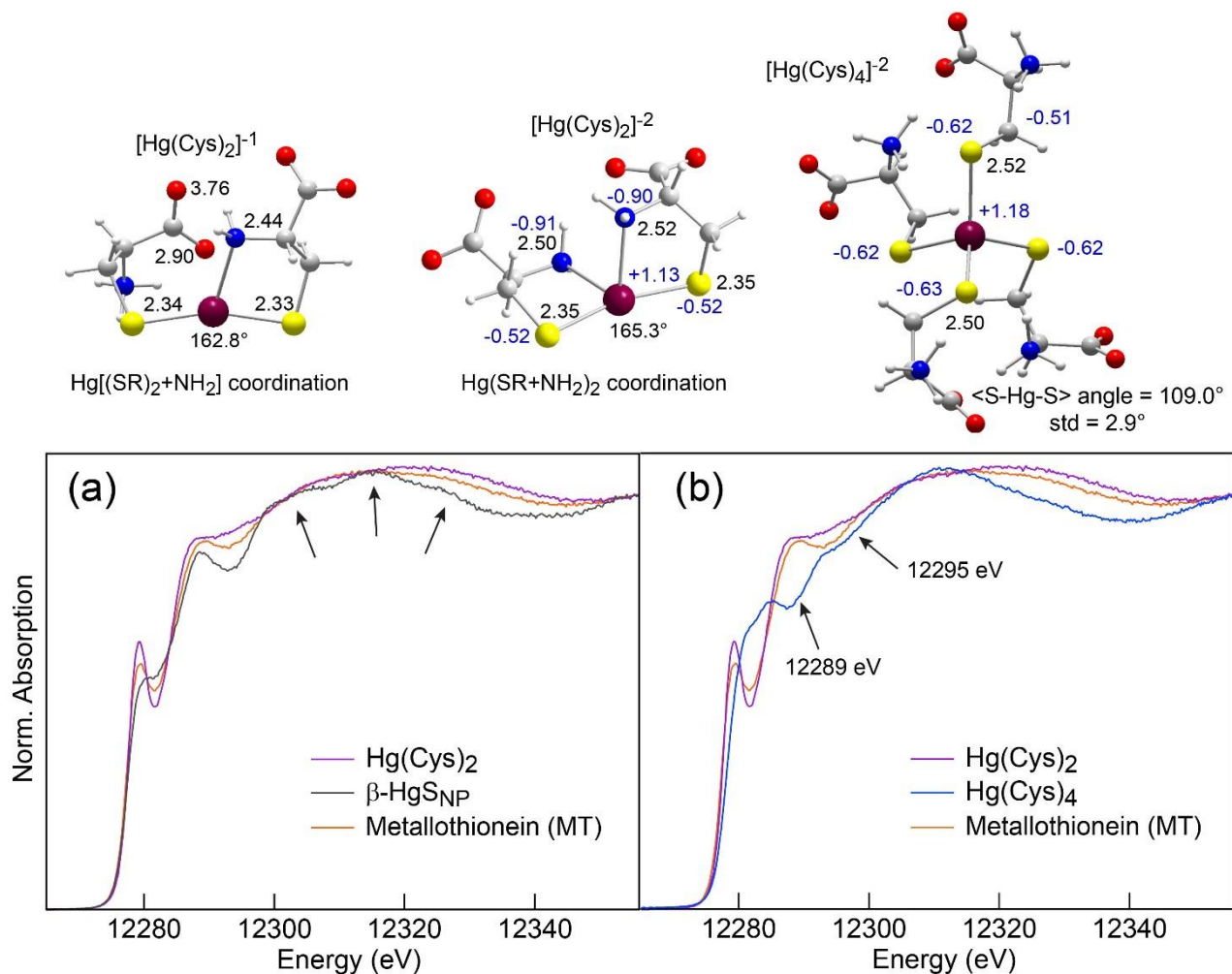
### 1. HR-XANES spectroscopy

The Hg L<sub>3</sub>-edge spectra were measured in high energy-resolution fluorescence yield detection mode with analyzer crystals.<sup>[1]</sup> Rejection of higher harmonics and reduction of heat load were achieved with a white beam Pd-coated, flat mirror working under total reflection at 2.5 mrad deflecting angle. The incoming beam was monochromatized by the 111 reflection of a Si double crystal monochromator, then focused horizontally by a second Pd-coated mirror and vertically by a third Pd-coated mirror. The flux on the sample was approximately 10<sup>13</sup> photons s<sup>-1</sup> in a beam footprint of ~700 (H) x 80 (V) μm<sup>2</sup> FWHM. The Hg L<sub>α1</sub> (3d<sub>5/2</sub> → 2p<sub>3/2</sub>) fluorescence line was selected using the 555 reflection of five spherically bent (radius = 0.5 m<sup>[2]</sup>) Si analyzer crystals (diameter = 100 mm) aligned at an 81.8° Bragg angle in a vertical Rowland geometry. The diffracted intensity was measured with a Si drift diode detector (SDD) in single photon counting mode. The effective energy resolution, obtained by convoluting the total instrument energy bandwidth (spreads of the incident and emitted rays), the SDD resolution (~160 eV), and the 3d<sub>5/2</sub> core-hole width from the L<sub>α1</sub> line was about 3.0 eV, compared to an intrinsic line broadening of about 6.1 eV in conventional fluorescence yield measurement with a solid-state detector.

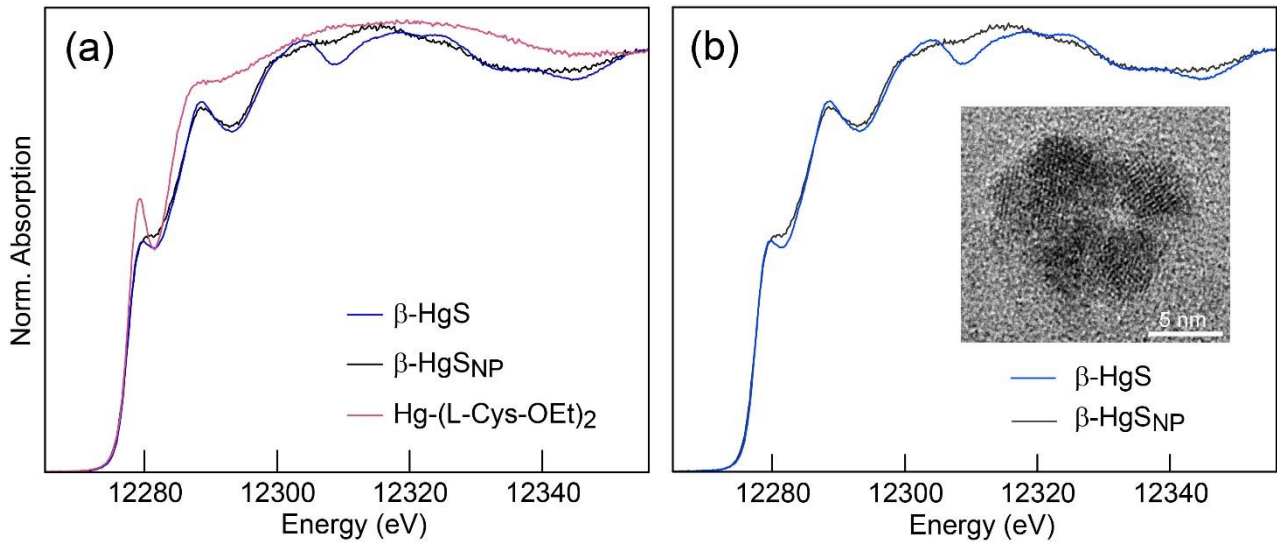
### 2. Supporting figures



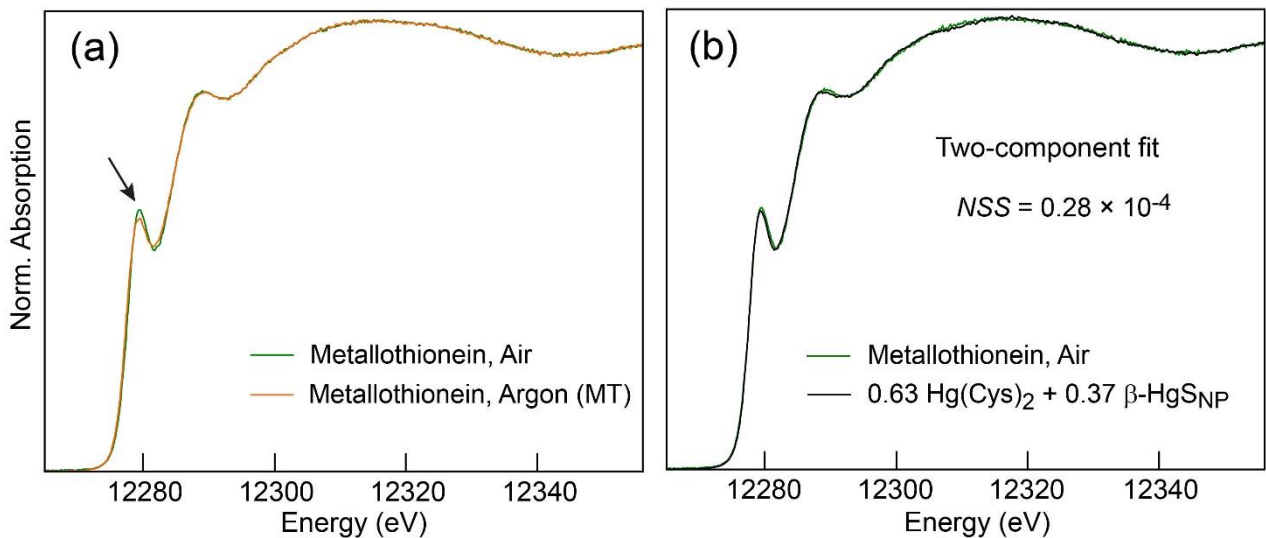
**Figure S1.** Space-filling representation of the mammalian Hg<sub>7</sub>-MT model optimized by Fowle and Stillman<sup>[3]</sup> using molecular mechanics (MM2). The Hg<sub>3</sub>S<sub>9</sub> cluster from the β domain is embedded within the peptide chain, whereas the bigger Hg<sub>4</sub>S<sub>11</sub> cluster is incompletely shielded from solvent by the protein. Thiolate groups exposed to the solvent at the MT surface (α domain) or in clefts (β domain) can establish intermolecular linkages between the monomeric units of the MT-20/30/40 oligomers through disulfide bonds.



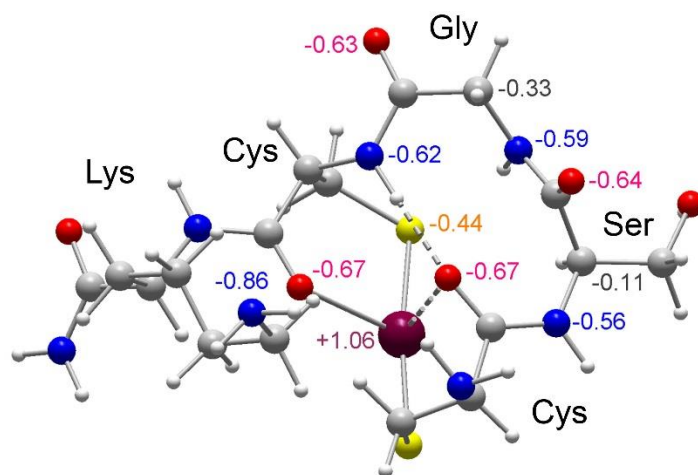
**Figure S2.** Mercury L<sub>3</sub>-edge HR-XANES spectra of metallothionein (MT) and three references relevant to this study: Hg(Cys)<sub>2</sub> complex in which Hg(II) is bonded linearly to two cysteines (Cys:Hg = 2.0, pH 7.5), Hg(Cys)<sub>4</sub> complex in which Hg(II) is bonded tetrahedrally to four cysteines (Cys:Hg = 10.0, pH 11.9), and nanoparticulate metacinnabar (β-HgS<sub>NP</sub>) in which Hg(II) is bonded to four sulfides (HgS<sub>4</sub>) and surrounded by Hg(II) atoms. The best two-component fit for the MT spectrum to a large dataset of references (ref.<sup>[4]</sup> and refs. therein) was obtained with Hg(Cys)<sub>2</sub> and β-HgS<sub>NP</sub> (Figure 5). A look at plot (a) confirms that the MT spectrum is intermediate between the two best-fit references. Plot (b) shows that the Hg(Cys)<sub>4</sub> reference provides a poor match to the MT spectrum. For example, the absorption signal of MT is close to that of Hg(Cys)<sub>2</sub> at 12289 eV and close to that of Hg(Cys)<sub>4</sub> at 12295 eV. Clearly, the MT spectrum cannot be reconstructed with a linear combination of a dithiolate and a mononuclear tetrathiolate environment. The XANES for β-HgS<sub>NP</sub> is structured by multiple scattering Hg-Hg paths of the photoelectron (arrows in plot (a)), in contrast to Hg(Cys)<sub>4</sub>. The two complexes were optimized geometrically (MP2/def2-TZVP-ecp<sup>[5]</sup>). At circumneutral pH, a Hg[(SR)<sub>2</sub>+NH<sub>2</sub>]<sub>2</sub> coordination likely coexists in equilibrium with the low-pH Hg(SR)<sub>2</sub> and the high-pH Hg(SR+NH<sub>2</sub>)<sub>2</sub> coordinations (see ref.<sup>[6]</sup> for details). Bond lengths (in angstroms) and bond angles are in black. Atomic charges, in units of elementary charge *e* and calculated by natural population analysis (NPA<sup>[7]</sup>) are in blue. Dark red, Hg; yellow, S; blue, N; red, O; gray, C; light gray, H.



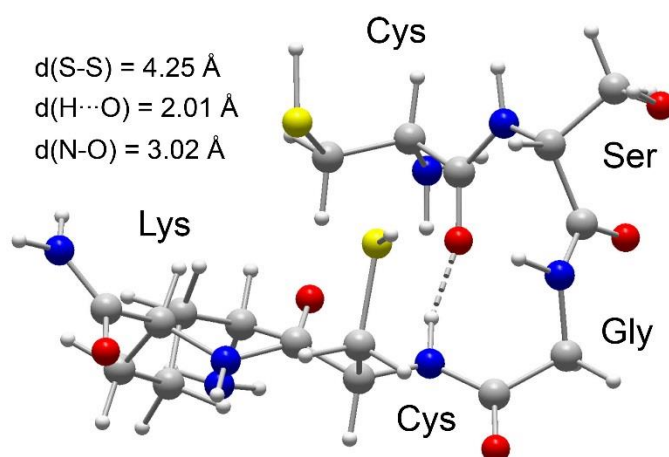
**Figure S3.** (a) Mercury L<sub>3</sub>-edge HR-XANES spectra of well ( $\beta$ -HgS) and nano ( $\beta$ -HgSNP) crystallized metacinnabar and the Hg-(L-Cys-OEt)<sub>2</sub> complex used to synthesize  $\beta$ -HgSNP. (b) The variations of the absorption signal in the main edge of  $\beta$ -HgS and  $\beta$ -HgSNP come from multiple scattering events along Hg<sub>1</sub> → Hg<sub>2</sub> ... Hg<sub>n</sub> → Hg<sub>1</sub> paths of the photoelectron. Structural disorder and small particle size reduce their amplitude. The spectra and the HRTEM image of the  $\beta$ -HgSNP crystallites in insert are from ref.<sup>[8]</sup>.



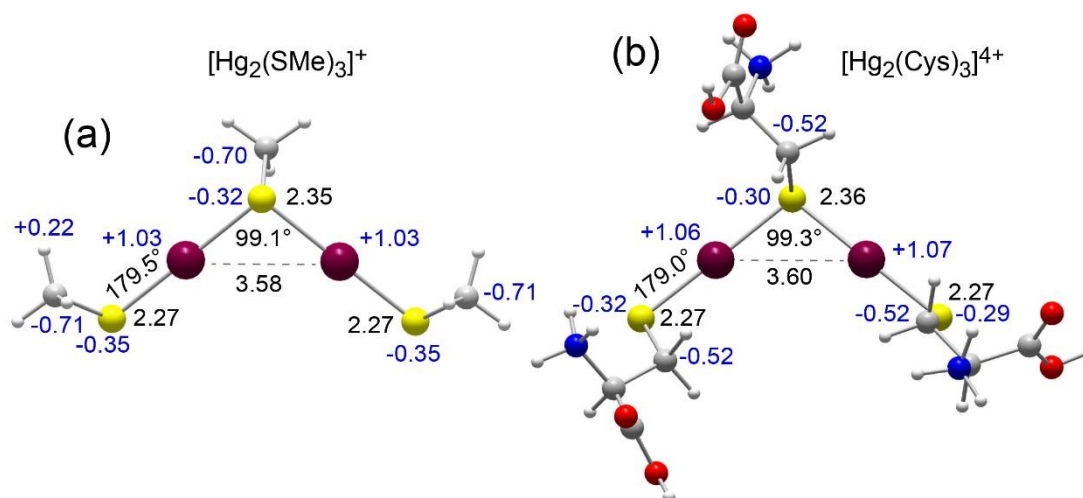
**Figure S4.** (a) Mercury L<sub>3</sub>-edge HR-XANES spectra of two MT isolates, one purified in argon-saturated and the other in air-equilibrated homogenate from mussel tissue. (b) Fit of the HR-XANES spectrum for the air-equilibrated MT.



**Figure S5.** Atomic charges in units of elementary charge  $e$  calculated by natural population analysis (NPA<sup>[7]</sup>) for the Hg(CysSerGlyCysLys) model complex. Dark red, Hg; yellow, S; blue, N; red, O; gray, C; light gray, H.

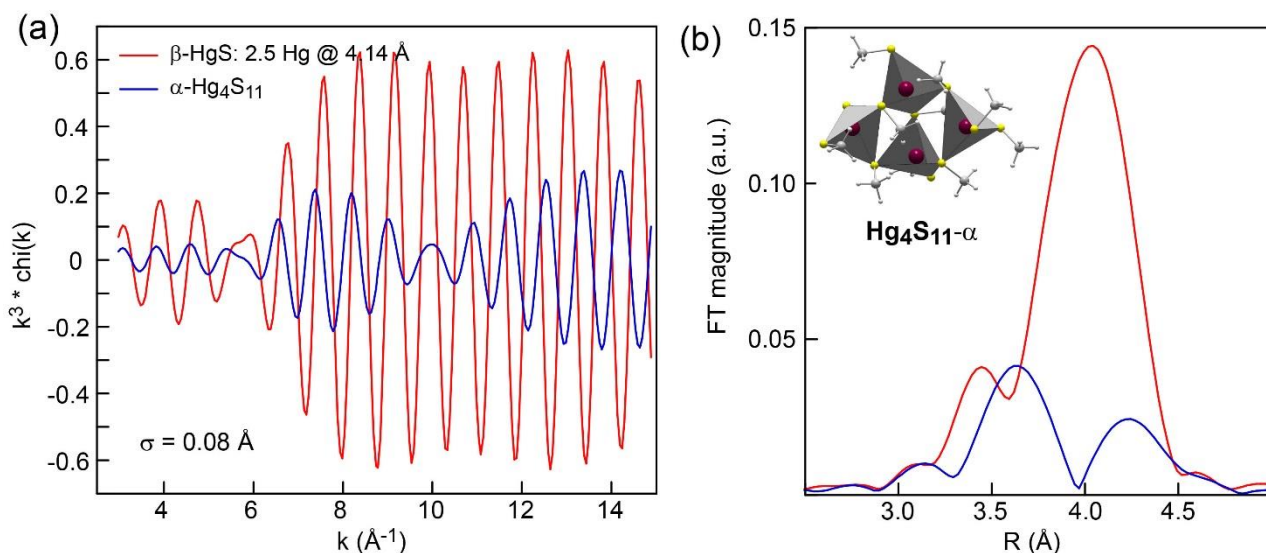


**Figure S6.** Geometry optimized (MP2/TZVP) crab claw shape of the CysSerGlyCysLys amino acid sequence of the  $\alpha$  domain. The two Cys residues lie above the quasi-planar CXXC loop stabilized by a  $>NH...OC<$  hydrogen bond. Mercury binding stabilizes the entire loop even further, giving it a very well-defined bis-six-membered ring chelate conformation (Figures 6b and S5).

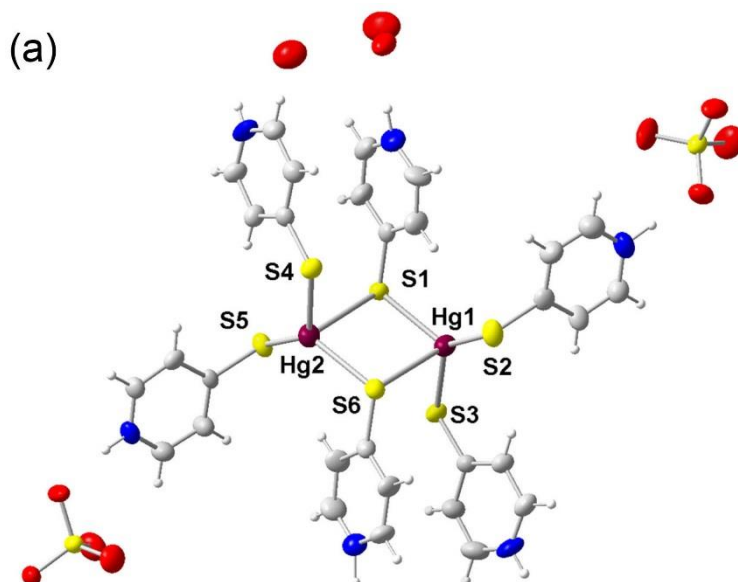


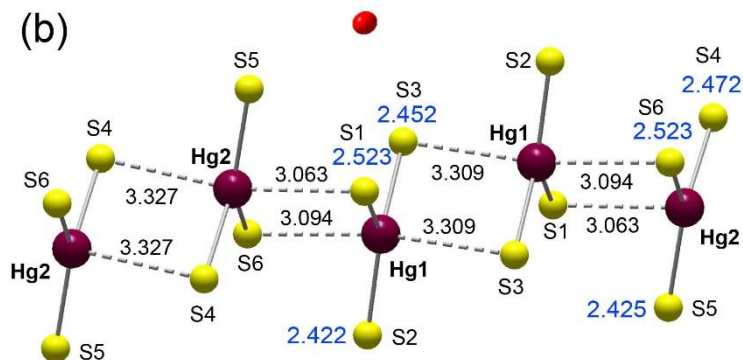


**Figure S7.** Geometry-optimized  $[\text{Hg}_2(\text{SMe})_3]^+$  (a) and  $[\text{Hg}_2(\text{Cys})_3]^{4+}$  (b) dimers (MP2/def2-TZVP-ecp<sup>[5]</sup>) and NPA<sup>[7]</sup> atomic charges (in blue and in units of elementary charge e). The cysteine group in the  $\text{Hg}_x\text{S}_y$  clusters from Figure 6 was represented by methanethiolate ( $\text{SCH}_3^- = \text{SMe}$ ) for simplification, as the dissociation energy of the R-SH bond is almost independent of R. We verify in this calculation that the methanethiolate for cysteinyl thiolate substitution does not alter the geometry of the complex nor change the partial atomic charges of Hg and S. Bond lengths (in angstroms) and bond angles are in black. Dark red, Hg; yellow, S; blue, N; red, O; gray, C; light gray, H.



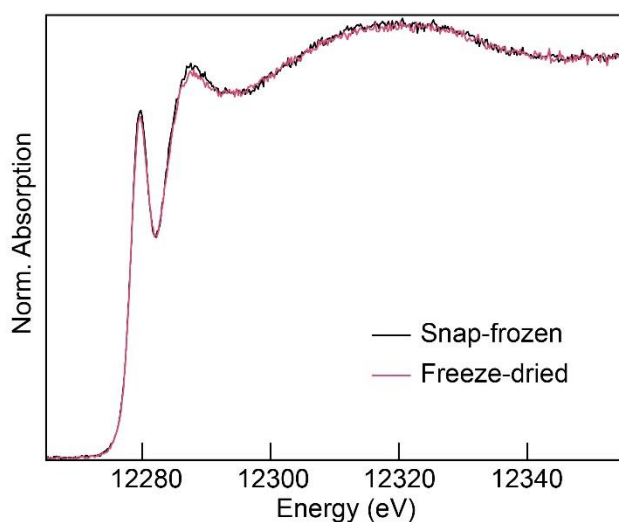
**Figure S8.** EXAFS photoelectron wave (a) and Fourier transform (b) of the first Hg-Hg shell for the  $\text{Hg}_4\text{S}_{11}\text{-}\alpha$  cluster.  $\langle \text{CN}(\text{Hg}) \rangle = 2.5$  and the predicted Hg-Hg distances are 3.82  $\text{\AA}$ , 4.05  $\text{\AA}$ , 4.20  $\text{\AA}$ , 4.24  $\text{\AA}$ , and 4.34  $\text{\AA}$  ( $\langle d(\text{Hg-Hg}) \rangle = 4.13$   $\text{\AA}$ ,  $\sigma = 0.19$   $\text{\AA}$ ).





**Figure S9.** (a) Representation of the  $[\text{Hg}_2(\text{C}_5\text{H}_5\text{NS})_6](\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$  asymmetric unit containing two crystallographic independent cationic  $[\text{Hg}(\text{C}_5\text{H}_5\text{NS})_3]^{2+}$  molecules. The Hg atoms are in a trigonal environment slightly off the mercapto planes ( $0.07 \text{ \AA}$  off S1, S2, S3 for Hg1 and  $0.05 \text{ \AA}$  off S4, S5, S6 for Hg2). The bond lengths (in  $\text{\AA}$ ) are Hg1-S1 =  $2.523(2)$ , Hg1-S2 =  $2.422(2)$ , Hg1-S3 =  $2.452(2)$ , Hg2-S4 =  $2.472(2)$ , Hg2-S5 =  $2.425(2)$ , Hg2-S6 =  $2.523(2)$ . (b) The coordination sphere of the Hg atoms is trigonal bipyramidal, with two apical S atoms from neighboring molecules resulting in linear chains. Linear chains are constituted of three types of  $\{\text{Hg-S-Hg-S}\}$  cycles. Two are centrosymmetric, one with  $d(\text{Hg1-S3}) = 3.309(2) \text{ \AA}$  and another with  $d(\text{Hg2-S4}) = 3.327(2) \text{ \AA}$ , leading to  $\text{Hg}\cdots\text{Hg}$  distances of  $3.898(2) \text{ \AA}$  and  $3.901(2) \text{ \AA}$ , respectively. The third is non-centrosymmetric with  $d(\text{Hg1-S6}) = 3.094(2) \text{ \AA}$  and  $d(\text{Hg2-S1}) = 3.063(2) \text{ \AA}$ , respectively, leading to a  $\text{Hg1}\cdots\text{Hg2}$  distance of  $3.889(2) \text{ \AA}$ . The chains are interconnected together by hydrogen bonds between pyridinium, sulfate anions and water molecules.

Two Cu(I) complexes with 4-mercaptopyridinium zwitterionic ligand have been reported<sup>[9]</sup>,  $[\text{Cu}(\text{C}_5\text{H}_5\text{NS})_4] \cdot 2\text{Cl}$  and  $[\text{Cu}(\text{C}_5\text{H}_5\text{NS})_4] \cdot \text{SiF}_6 \cdot 2\text{MeOH}$ , which have similar formula to  $[\text{Hg}_2(\text{C}_5\text{H}_5\text{NS})_6](\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ . In contrast to the Hg complex, the structures feature centrosymmetric binuclear complexes and the Cu(I) atoms are four-coordinate with average Cu-S bond lengths of  $2.40 \text{ \AA}$  and  $2.30 \text{ \AA}$  for the bridging and terminal ligands, respectively.



**Figure S10.** Mercury  $L_3$ -edge HR-XANES spectra of swordfish skeletal muscle prepared in two different ways: by snap-freezing a fresh hydrated tissue and by freeze-drying and pressing ( $444 \text{ MPa}$ ) into a pellet a frozen tissue. The sharp near-edge structure is a fingerprint for the  $\text{CH}_3\text{-Hg-SR}$  bond of methylmercury complexed to biological cysteine residues from peptide or protein.<sup>[6]</sup> The identity of the two spectra, within the noise, means that the  $\text{Hg(II)-CH}_3$  and the  $\text{Hg(II)-SR}$  bonds both resisted dehydration under vacuum and moderate pressure.

### 3. References

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### 4. HR-XANES data

ME	MT_Air	T_Argon
1.2258820E+4 3.0583329E-4	1.2258820E+4 4.7706828E-3	1.2258820E+4 1.2431541E-3
1.2258840E+4 3.0998651E-4	1.2258840E+4 4.6142566E-3	1.2258840E+4 1.2447467E-3
1.2258980E+4 3.3366120E-4	1.2258980E+4 3.2354888E-3	1.2258980E+4 1.3511280E-3
1.2259200E+4 3.8925987E-4	1.2259200E+4 3.8754295E-3	1.2259200E+4 1.2498947E-3
1.2259410E+4 3.6761042E-4	1.2259410E+4 4.2808968E-3	1.2259410E+4 8.0460482E-4
1.2259620E+4 3.0252888E-4	1.2259620E+4 4.2046641E-3	1.2259620E+4 1.1854319E-3
1.2259820E+4 4.1355212E-4	1.2259820E+4 4.6939334E-3	1.2259820E+4 1.6527924E-3
1.2260020E+4 4.3025388E-4	1.2260020E+4 3.0387831E-3	1.2260020E+4 1.3072032E-3
1.2260210E+4 3.8933738E-4	1.2260210E+4 2.8396122E-3	1.2260210E+4 2.2397377E-3
1.2260400E+4 3.8992397E-4	1.2260400E+4 4.3375014E-3	1.2260400E+4 1.6755351E-3
1.2260590E+4 3.8906836E-4	1.2260590E+4 2.0150138E-3	1.2260590E+4 1.2467509E-3
1.2260800E+4 4.1840826E-4	1.2260800E+4 2.6833678E-3	1.2260800E+4 1.0295534E-3
1.2261020E+4 4.1715896E-4	1.2261020E+4 2.5597407E-3	1.2261020E+4 8.6439926E-4
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1.2261440E+4 3.4990951E-4	1.2261440E+4 1.6033309E-3	1.2261440E+4 1.0929317E-3
1.2261630E+4 4.5888778E-4	1.2261630E+4 2.7020289E-3	1.2261630E+4 1.0555090E-3
1.2261830E+4 4.0060784E-4	1.2261830E+4 3.9250955E-3	1.2261830E+4 2.2850732E-3
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1.2262390E+4 4.8661522E-4	1.2262390E+4 3.8432095E-3	1.2262390E+4 1.8815522E-3
1.2262600E+4 5.4754891E-4	1.2262600E+4 2.3637395E-3	1.2262600E+4 2.1142196E-3
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1.2263000E+4 4.7539470E-4	1.2263000E+4 4.4867154E-3	1.2263000E+4 1.5215665E-3
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1.2263710E+4 5.6084426E-4	1.2263710E+4 1.6720996E-3	1.2263710E+4 1.5826387E-3
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1.2264080E+4 7.1657210E-4	1.2264080E+4 2.6750279E-3	1.2264080E+4 9.0059914E-4



1.2264270E+4 6.3702252E-4	1.2264270E+4 2.7946050E-3	1.2264270E+4 1.3629147E-3
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1.2265020E+4 8.1488964E-4	1.2265020E+4 2.1661577E-3	1.2265020E+4 7.4901380E-5
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1.2271010E+4 3.1235366E-3	1.2271010E+4 6.7167023E-3	1.2271010E+4 2.5397179E-3
1.2271220E+4 3.5442623E-3	1.2271220E+4 5.9532763E-3	1.2271220E+4 3.1989704E-3
1.2271410E+4 3.7675515E-3	1.2271410E+4 6.0948678E-3	1.2271410E+4 4.2480432E-3
1.2271590E+4 3.8976699E-3	1.2271590E+4 6.8000174E-3	1.2271590E+4 4.1021279E-3
1.2271780E+4 4.3751929E-3	1.2271780E+4 5.6278626E-3	1.2271780E+4 4.2730832E-3
1.2272000E+4 4.9506634E-3	1.2272000E+4 6.5504545E-3	1.2272000E+4 6.0025731E-3
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1.2272430E+4 5.9126626E-3	1.2272430E+4 7.3743560E-3	1.2272430E+4 5.9496739E-3
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1.2272830E+4 7.5042364E-3	1.2272830E+4 9.4719330E-3	1.2272830E+4 8.2838555E-3
1.2273020E+4 8.2830410E-3	1.2273020E+4 1.0004011E-2	1.2273020E+4 8.7471249E-3
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1.2273600E+4 1.1815860E-2	1.2273600E+4 1.5146019E-2	1.2273600E+4 1.4270868E-2
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1.2274020E+4 1.6094838E-2	1.2274020E+4 1.9431084E-2	1.2274020E+4 1.9175043E-2
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1.2327260E+4	1.0575888E+0	1.2327260E+4	1.0374523E+0	1.2327260E+4	1.0373250E+0
1.2327480E+4	1.0578091E+0	1.2327480E+4	1.0398140E+0	1.2327480E+4	1.0379171E+0
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1.2328870E+4	1.0503664E+0	1.2328870E+4	1.0328348E+0	1.2328870E+4	1.0331360E+0
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1.2331560E+4	1.0409314E+0	1.2331560E+4	1.0235545E+0	1.2331560E+4	1.0190192E+0
1.2331780E+4	1.0392725E+0	1.2331780E+4	1.0177817E+0	1.2331780E+4	1.0181040E+0
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1.2332990E+4	1.0323557E+0	1.2332990E+4	1.0105715E+0	1.2332990E+4	1.0087994E+0
1.2333170E+4	1.0322902E+0	1.2333170E+4	1.0106408E+0	1.2333170E+4	1.0112759E+0
1.2333360E+4	1.0323339E+0	1.2333360E+4	1.0061074E+0	1.2333360E+4	1.0044337E+0
1.2333560E+4	1.0319215E+0	1.2333560E+4	1.0057464E+0	1.2333560E+4	1.0041246E+0
1.2333760E+4	1.0298286E+0	1.2333760E+4	1.0051623E+0	1.2333760E+4	1.0055600E+0
1.2333970E+4	1.0306657E+0	1.2333970E+4	1.0055712E+0	1.2333970E+4	1.0068441E+0
1.2334160E+4	1.0284425E+0	1.2334160E+4	1.0128530E+0	1.2334160E+4	1.0087460E+0
1.2334350E+4	1.0272418E+0	1.2334350E+4	1.0066115E+0	1.2334350E+4	1.0056910E+0
1.2334530E+4	1.0274471E+0	1.2334530E+4	1.0055893E+0	1.2334530E+4	1.0012200E+0
1.2334710E+4	1.0254895E+0	1.2334710E+4	1.0096957E+0	1.2334710E+4	1.0057211E+0
1.2334900E+4	1.0263488E+0	1.2334900E+4	1.0062994E+0	1.2334900E+4	1.0076563E+0
1.2335110E+4	1.0266124E+0	1.2335110E+4	1.0030083E+0	1.2335110E+4	1.0030602E+0
1.2335320E+4	1.0234620E+0	1.2335320E+4	1.0005667E+0	1.2335320E+4	1.0047334E+0
1.2335540E+4	1.0240463E+0	1.2335540E+4	1.0041494E+0	1.2335540E+4	1.0010849E+0
1.2335750E+4	1.0208211E+0	1.2335750E+4	9.9867785E-1	1.2335750E+4	9.9823857E-1
1.2335960E+4	1.0189343E+0	1.2335960E+4	1.0014430E+0	1.2335960E+4	9.9926917E-1
1.2336160E+4	1.0192068E+0	1.2336160E+4	9.9964700E-1	1.2336160E+4	9.9753945E-1
1.2336360E+4	1.0201388E+0	1.2336360E+4	1.0000941E+0	1.2336360E+4	9.9591291E-1

1.2336560E+4 1.0189816E+0	1.2336560E+4 9.9821664E-1	1.2336560E+4 9.9542987E-1
1.2336760E+4 1.0175689E+0	1.2336760E+4 9.9768197E-1	1.2336760E+4 9.9397788E-1
1.2336980E+4 1.0129309E+0	1.2336980E+4 9.9475454E-1	1.2336980E+4 9.9405720E-1
1.2337200E+4 1.0124510E+0	1.2337200E+4 9.9272140E-1	1.2337200E+4 9.9590253E-1
1.2337410E+4 1.0138346E+0	1.2337410E+4 9.9145871E-1	1.2337410E+4 9.9371052E-1
1.2337620E+4 1.0135358E+0	1.2337620E+4 9.9026165E-1	1.2337620E+4 9.9195160E-1
1.2337810E+4 1.0144906E+0	1.2337810E+4 9.9356114E-1	1.2337810E+4 9.9672924E-1
1.2338010E+4 1.0129975E+0	1.2338010E+4 9.9057964E-1	1.2338010E+4 9.9220122E-1
1.2338190E+4 1.0115725E+0	1.2338190E+4 9.8672505E-1	1.2338190E+4 9.8934959E-1
1.2338390E+4 1.0095931E+0	1.2338390E+4 9.9169796E-1	1.2338390E+4 9.8812710E-1
1.2338590E+4 1.0091301E+0	1.2338590E+4 9.9102405E-1	1.2338590E+4 9.8921418E-1
1.2338800E+4 1.0097937E+0	1.2338800E+4 9.8660095E-1	1.2338800E+4 9.8385201E-1
1.2339010E+4 1.0086561E+0	1.2339010E+4 9.8752635E-1	1.2339010E+4 9.8729146E-1
1.2339210E+4 1.0070642E+0	1.2339210E+4 9.9209235E-1	1.2339210E+4 9.8785233E-1
1.2339420E+4 1.0060965E+0	1.2339420E+4 9.8253112E-1	1.2339420E+4 9.8429783E-1
1.2339620E+4 1.0054891E+0	1.2339620E+4 9.8514775E-1	1.2339620E+4 9.8804048E-1
1.2339810E+4 1.0045933E+0	1.2339810E+4 9.8610096E-1	1.2339810E+4 9.8456681E-1
1.2340000E+4 1.0028930E+0	1.2340000E+4 9.8712625E-1	1.2340000E+4 9.8332471E-1
1.2340210E+4 1.0052281E+0	1.2340210E+4 9.8031951E-1	1.2340210E+4 9.8007715E-1
1.2340410E+4 1.0041829E+0	1.2340410E+4 9.8271394E-1	1.2340410E+4 9.7742952E-1
1.2340630E+4 1.0023744E+0	1.2340630E+4 9.8330975E-1	1.2340630E+4 9.8544344E-1
1.2340840E+4 1.0019695E+0	1.2340840E+4 9.8292584E-1	1.2340840E+4 9.8134029E-1
1.2341040E+4 1.0007605E+0	1.2341040E+4 9.8622967E-1	1.2341040E+4 9.8437025E-1
1.2341230E+4 9.9904455E-1	1.2341230E+4 9.8346472E-1	1.2341230E+4 9.8386855E-1
1.2341420E+4 9.9841996E-1	1.2341420E+4 9.7972353E-1	1.2341420E+4 9.8000008E-1
1.2341600E+4 1.0013552E+0	1.2341600E+4 9.8046093E-1	1.2341600E+4 9.8156929E-1
1.2341790E+4 9.9835459E-1	1.2341790E+4 9.8156279E-1	1.2341790E+4 9.8283162E-1
1.2341980E+4 9.9964437E-1	1.2341980E+4 9.8051423E-1	1.2341980E+4 9.8273133E-1
1.2342190E+4 9.9706640E-1	1.2342190E+4 9.7906667E-1	1.2342190E+4 9.7758266E-1
1.2342390E+4 9.9784751E-1	1.2342390E+4 9.7526095E-1	1.2342390E+4 9.7844384E-1
1.2342580E+4 9.9510461E-1	1.2342580E+4 9.7666481E-1	1.2342580E+4 9.7651009E-1
1.2342770E+4 9.9830377E-1	1.2342770E+4 9.7975727E-1	1.2342770E+4 9.7898445E-1
1.2342950E+4 9.9664689E-1	1.2342950E+4 9.7327629E-1	1.2342950E+4 9.7654840E-1
1.2343130E+4 9.9561455E-1	1.2343130E+4 9.7830861E-1	1.2343130E+4 9.7823322E-1
1.2343310E+4 9.9525900E-1	1.2343310E+4 9.8146132E-1	1.2343310E+4 9.7595974E-1
1.2343500E+4 9.9628672E-1	1.2343500E+4 9.7418018E-1	1.2343500E+4 9.7795439E-1
1.2343690E+4 9.9464939E-1	1.2343690E+4 9.8101915E-1	1.2343690E+4 9.8176950E-1
1.2343900E+4 9.9226039E-1	1.2343900E+4 9.7748250E-1	1.2343900E+4 9.7810173E-1
1.2344110E+4 9.9680889E-1	1.2344110E+4 9.8471097E-1	1.2344110E+4 9.8068837E-1
1.2344310E+4 9.9712347E-1	1.2344310E+4 9.7918895E-1	1.2344310E+4 9.7785390E-1
1.2344500E+4 9.9306113E-1	1.2344500E+4 9.8250233E-1	1.2344500E+4 9.7875269E-1
1.2344680E+4 9.9204686E-1	1.2344680E+4 9.7774683E-1	1.2344680E+4 9.7300106E-1
1.2344860E+4 9.9089516E-1	1.2344860E+4 9.7904017E-1	1.2344860E+4 9.7777919E-1
1.2345060E+4 9.9194423E-1	1.2345060E+4 9.7704088E-1	1.2345060E+4 9.8055791E-1
1.2345280E+4 9.9274516E-1	1.2345280E+4 9.8018596E-1	1.2345280E+4 9.7742813E-1
1.2345500E+4 9.9230412E-1	1.2345500E+4 9.7638891E-1	1.2345500E+4 9.7705199E-1
1.2345710E+4 9.9322451E-1	1.2345710E+4 9.7778733E-1	1.2345710E+4 9.7620503E-1
1.2345910E+4 9.9272763E-1	1.2345910E+4 9.8461807E-1	1.2345910E+4 9.8399346E-1
1.2346110E+4 9.9268105E-1	1.2346110E+4 9.7791740E-1	1.2346110E+4 9.8022676E-1
1.2346290E+4 9.9302454E-1	1.2346290E+4 9.7792754E-1	1.2346290E+4 9.7509184E-1
1.2346480E+4 9.9321681E-1	1.2346480E+4 9.7679924E-1	1.2346480E+4 9.7522117E-1
1.2346670E+4 9.9450929E-1	1.2346670E+4 9.7818980E-1	1.2346670E+4 9.7945529E-1

1.2346870E+4 9.9293896E-1	1.2346870E+4 9.7964870E-1	1.2346870E+4 9.8169704E-1
1.2347070E+4 9.8947737E-1	1.2347070E+4 9.7888243E-1	1.2347070E+4 9.7733161E-1
1.2347270E+4 9.9185641E-1	1.2347270E+4 9.8075624E-1	1.2347270E+4 9.7651833E-1
1.2347460E+4 9.9243095E-1	1.2347460E+4 9.8317900E-1	1.2347460E+4 9.8173540E-1
1.2347650E+4 9.9074424E-1	1.2347650E+4 9.8214815E-1	1.2347650E+4 9.8283047E-1
1.2347840E+4 9.9355198E-1	1.2347840E+4 9.8125352E-1	1.2347840E+4 9.8218139E-1
1.2348020E+4 9.9288781E-1	1.2348020E+4 9.8280781E-1	1.2348020E+4 9.8311773E-1
1.2348210E+4 9.9149136E-1	1.2348210E+4 9.8129670E-1	1.2348210E+4 9.8179521E-1
1.2348420E+4 9.9419959E-1	1.2348420E+4 9.7949782E-1	1.2348420E+4 9.8147800E-1
1.2348630E+4 9.9135333E-1	1.2348630E+4 9.8303853E-1	1.2348630E+4 9.8023942E-1
1.2348860E+4 9.9387122E-1	1.2348860E+4 9.8043237E-1	1.2348860E+4 9.8144727E-1
1.2349070E+4 9.9199231E-1	1.2349070E+4 9.8115537E-1	1.2349070E+4 9.8296879E-1
1.2349280E+4 9.9212956E-1	1.2349280E+4 9.8052671E-1	1.2349280E+4 9.8209890E-1
1.2349490E+4 9.9509037E-1	1.2349490E+4 9.8579353E-1	1.2349490E+4 9.8439616E-1
1.2349680E+4 9.9243445E-1	1.2349680E+4 9.8253638E-1	1.2349680E+4 9.7971767E-1
1.2349890E+4 9.9331037E-1	1.2349890E+4 9.8623289E-1	1.2349890E+4 9.8666731E-1
1.2350090E+4 9.9482356E-1	1.2350090E+4 9.8505086E-1	1.2350090E+4 9.8262646E-1
1.2350300E+4 9.9398328E-1	1.2350300E+4 9.8327961E-1	1.2350300E+4 9.8473528E-1
1.2350530E+4 9.9600321E-1	1.2350530E+4 9.8541907E-1	1.2350530E+4 9.8643845E-1
1.2350740E+4 9.9494426E-1	1.2350740E+4 9.8156681E-1	1.2350740E+4 9.8622522E-1
1.2350950E+4 9.9563721E-1	1.2350950E+4 9.8590313E-1	1.2350950E+4 9.8824698E-1
1.2351160E+4 9.9382787E-1	1.2351160E+4 9.8599556E-1	1.2351160E+4 9.8858092E-1
1.2351360E+4 9.9640713E-1	1.2351360E+4 9.8635748E-1	1.2351360E+4 9.8937597E-1
1.2351550E+4 9.9519387E-1	1.2351550E+4 9.8790327E-1	1.2351550E+4 9.9279249E-1
1.2351740E+4 9.9299445E-1	1.2351740E+4 9.8756443E-1	1.2351740E+4 9.8966154E-1
1.2351960E+4 9.9621487E-1	1.2351960E+4 9.9100936E-1	1.2351960E+4 9.8785156E-1
1.2352180E+4 9.9968776E-1	1.2352180E+4 9.9035569E-1	1.2352180E+4 9.9072385E-1
1.2352400E+4 9.9922425E-1	1.2352400E+4 9.9284900E-1	1.2352400E+4 9.9559576E-1
1.2352620E+4 9.9681556E-1	1.2352620E+4 9.9474020E-1	1.2352620E+4 9.8985442E-1
1.2352820E+4 9.9634893E-1	1.2352820E+4 9.9835969E-1	1.2352820E+4 9.9690266E-1
1.2353030E+4 9.9670803E-1	1.2353030E+4 9.9216016E-1	1.2353030E+4 9.9761034E-1
1.2353230E+4 9.9752032E-1	1.2353230E+4 9.9243256E-1	1.2353230E+4 9.9576073E-1
1.2353420E+4 9.9705096E-1	1.2353420E+4 9.9578970E-1	1.2353420E+4 9.9503840E-1
1.2353620E+4 9.9778566E-1	1.2353620E+4 9.9623553E-1	1.2353620E+4 9.9591187E-1
1.2353840E+4 9.9985016E-1	1.2353840E+4 9.9625804E-1	1.2353840E+4 9.9764633E-1
1.2354060E+4 9.9781150E-1	1.2354060E+4 9.9860486E-1	1.2354060E+4 9.9224776E-1
1.2354290E+4 1.0003358E+0	1.2354290E+4 9.9831207E-1	1.2354290E+4 9.9644384E-1
1.2354500E+4 1.0002729E+0	1.2354500E+4 9.9827390E-1	1.2354500E+4 9.9836835E-1
1.2354690E+4 1.0009214E+0	1.2354690E+4 9.9800786E-1	1.2354690E+4 9.9974658E-1
1.2354890E+4 1.0012992E+0	1.2354890E+4 9.9644333E-1	1.2354890E+4 9.9826318E-1
1.2355070E+4 1.0000086E+0	1.2355070E+4 9.9656321E-1	1.2355070E+4 9.9943193E-1
1.2355270E+4 9.9885785E-1	1.2355270E+4 1.0014159E+0	1.2355270E+4 1.0028662E+0
1.2355470E+4 1.0003480E+0	1.2355470E+4 9.9937360E-1	1.2355470E+4 9.9775050E-1
1.2355680E+4 1.0009893E+0	1.2355680E+4 9.9984666E-1	1.2355680E+4 9.9863572E-1
1.2355890E+4 1.0002001E+0	1.2355890E+4 1.0032062E+0	1.2355890E+4 1.0004873E+0
1.2356080E+4 1.0014147E+0	1.2356080E+4 1.0022079E+0	1.2356080E+4 1.0009022E+0
1.2356280E+4 1.0033571E+0	1.2356280E+4 1.0031780E+0	1.2356280E+4 1.0060698E+0
1.2356470E+4 1.0036077E+0	1.2356470E+4 1.0016097E+0	1.2356470E+4 1.0012426E+0

**Hg(Cys)<sub>2</sub>**

1.2258820E+4 8.3837000E-5  
1.2258840E+4 3.3173000E-4

**β-HgS nano**

1.2258820E+4 7.4837000E-4  
1.2258840E+4 9.3373000E-4

**Hg(D-Pen)<sub>3</sub>**

1.2258820E+4 1.4094051E-3  
1.2258840E+4 1.4469796E-3

1.2258980E+4	2.1279000E-4	1.2258980E+4	1.0480111E-3	1.2258980E+4	1.5649153E-3
1.2259200E+4	1.0806131E-4	1.2259200E+4	1.0746625E-3	1.2259200E+4	1.7787419E-3
1.2259410E+4	3.3996248E-4	1.2259410E+4	7.9168076E-4	1.2259410E+4	2.7566629E-3
1.2259620E+4	1.2829205E-5	1.2259620E+4	1.0113411E-3	1.2259620E+4	3.2614877E-3
1.2259820E+4	9.3999756E-5	1.2259820E+4	7.1882701E-4	1.2259820E+4	2.1856813E-3
1.2260020E+4	1.1576236E-4	1.2260020E+4	1.5482408E-3	1.2260020E+4	3.2974770E-3
1.2260210E+4	1.0606810E-4	1.2260210E+4	1.7437281E-3	1.2260210E+4	2.6823506E-3
1.2260400E+4	2.1074166E-4	1.2260400E+4	1.5301288E-3	1.2260400E+4	3.5986510E-3
1.2260590E+4	2.0437958E-4	1.2260590E+4	1.5656518E-3	1.2260590E+4	3.2185234E-3
1.2260800E+4	2.2199840E-4	1.2260800E+4	1.1236553E-3	1.2260800E+4	2.0690490E-3
1.2261020E+4	4.1591612E-4	1.2261020E+4	1.1639942E-3	1.2261020E+4	2.1650826E-3
1.2261230E+4	3.5458021E-4	1.2261230E+4	2.3113683E-3	1.2261230E+4	2.5409028E-3
1.2261440E+4	1.0840559E-4	1.2261440E+4	1.4042381E-3	1.2261440E+4	1.8792836E-3
1.2261630E+4	1.4135220E-4	1.2261630E+4	1.1529419E-3	1.2261630E+4	2.8459113E-3
1.2261830E+4	3.6705337E-4	1.2261830E+4	1.7243508E-3	1.2261830E+4	1.8850000E-3
1.2262010E+4	3.0660441E-4	1.2262010E+4	1.3617432E-3	1.2262010E+4	2.9058000E-3
1.2262190E+4	1.8654197E-4	1.2262190E+4	1.0170524E-3	1.2262190E+4	2.6259090E-3
1.2262390E+4	3.9235229E-4	1.2262390E+4	1.2283104E-3	1.2262390E+4	2.1360701E-3
1.2262600E+4	1.4877210E-4	1.2262600E+4	1.8635973E-3	1.2262600E+4	2.9850000E-3
1.2262800E+4	2.8664541E-4	1.2262800E+4	1.9897571E-3	1.2262800E+4	2.8267415E-3
1.2263000E+4	1.7777159E-4	1.2263000E+4	2.0806461E-3	1.2263000E+4	2.4215131E-3
1.2263190E+4	4.9879103E-4	1.2263190E+4	1.8615567E-3	1.2263190E+4	2.1208458E-3
1.2263370E+4	5.0500295E-4	1.2263370E+4	1.6264101E-3	1.2263370E+4	2.5331365E-3
1.2263540E+4	3.8587011E-4	1.2263540E+4	1.8941674E-3	1.2263540E+4	3.2003001E-3
1.2263710E+4	5.6627598E-4	1.2263710E+4	1.9634409E-3	1.2263710E+4	2.6329947E-3
1.2263890E+4	5.8006639E-4	1.2263890E+4	1.8580563E-3	1.2263890E+4	2.6666334E-3
1.2264080E+4	3.8308808E-4	1.2264080E+4	1.8694992E-3	1.2264080E+4	2.7828830E-3
1.2264270E+4	4.1860969E-4	1.2264270E+4	7.2147440E-4	1.2264270E+4	2.8237719E-3
1.2264460E+4	4.7993268E-4	1.2264460E+4	2.0741522E-3	1.2264460E+4	2.4075970E-3
1.2264660E+4	4.9181844E-4	1.2264660E+4	1.7808624E-3	1.2264660E+4	2.3090434E-3
1.2264840E+4	4.7780188E-4	1.2264840E+4	2.1087284E-3	1.2264840E+4	2.4704374E-3
1.2265020E+4	5.9537774E-4	1.2265020E+4	2.1744903E-3	1.2265020E+4	3.0850997E-3
1.2265200E+4	5.8191326E-4	1.2265200E+4	2.0018826E-3	1.2265200E+4	3.7463502E-3
1.2265390E+4	1.8852709E-4	1.2265390E+4	1.3810956E-3	1.2265390E+4	3.0047366E-3
1.2265590E+4	3.3224945E-4	1.2265590E+4	1.6173571E-3	1.2265590E+4	2.7780708E-3
1.2265790E+4	3.9535181E-4	1.2265790E+4	1.6323552E-3	1.2265790E+4	2.4407131E-3
1.2265990E+4	4.2675930E-4	1.2265990E+4	2.0548243E-3	1.2265990E+4	2.2955672E-3
1.2266190E+4	5.8530001E-4	1.2266190E+4	2.1031420E-3	1.2266190E+4	3.1970054E-3
1.2266380E+4	8.0116414E-4	1.2266380E+4	2.0195610E-3	1.2266380E+4	2.9953120E-3
1.2266560E+4	7.5553683E-4	1.2266560E+4	1.8629950E-3	1.2266560E+4	2.4011450E-3
1.2266740E+4	8.6869404E-4	1.2266740E+4	1.1199453E-3	1.2266740E+4	2.2454555E-3
1.2266920E+4	8.7162578E-4	1.2266920E+4	1.7443707E-3	1.2266920E+4	2.7022522E-3
1.2267110E+4	1.0764250E-3	1.2267110E+4	2.6046088E-3	1.2267110E+4	3.0134958E-3
1.2267310E+4	7.7488147E-4	1.2267310E+4	2.6537737E-3	1.2267310E+4	3.5385972E-3
1.2267500E+4	8.2549930E-4	1.2267500E+4	2.3937965E-3	1.2267500E+4	3.4918563E-3
1.2267700E+4	1.2216445E-3	1.2267700E+4	1.6595609E-3	1.2267700E+4	2.2554567E-3
1.2267880E+4	1.0522527E-3	1.2267880E+4	1.8352068E-3	1.2267880E+4	2.9069318E-3
1.2268060E+4	1.2015254E-3	1.2268060E+4	1.6565366E-3	1.2268060E+4	4.1722000E-3
1.2268230E+4	9.8594448E-4	1.2268230E+4	1.9811271E-3	1.2268230E+4	3.5485918E-3
1.2268410E+4	1.2043601E-3	1.2268410E+4	2.1524073E-3	1.2268410E+4	4.0615616E-3
1.2268590E+4	1.2191272E-3	1.2268590E+4	2.6552772E-3	1.2268590E+4	3.5864402E-3
1.2268790E+4	1.4179481E-3	1.2268790E+4	2.6244996E-3	1.2268790E+4	2.6523219E-3

1.2268990E+4 1.5647530E-3	1.2268990E+4 2.8994277E-3	1.2268990E+4 2.6803078E-3
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1.2295900E+4 9.3702244E-1 1.2295900E+4 8.6972057E-1 1.2295900E+4 8.8647710E-1  
1.2296100E+4 9.3329183E-1 1.2296100E+4 8.8208039E-1 1.2296100E+4 8.9108528E-1  
1.2296300E+4 9.3495226E-1 1.2296300E+4 8.8986418E-1 1.2296300E+4 8.9562166E-1  
1.2296490E+4 9.3616373E-1 1.2296490E+4 8.9820201E-1 1.2296490E+4 9.0020078E-1  
1.2296690E+4 9.4097779E-1 1.2296690E+4 9.0531005E-1 1.2296690E+4 9.0015833E-1  
1.2296900E+4 9.3949078E-1 1.2296900E+4 9.1289328E-1 1.2296900E+4 9.0528493E-1  
1.2297130E+4 9.4078577E-1 1.2297130E+4 9.2007316E-1 1.2297130E+4 9.0736761E-1  
1.2297350E+4 9.4811062E-1 1.2297350E+4 9.2478358E-1 1.2297350E+4 9.1126649E-1  
1.2297550E+4 9.4749798E-1 1.2297550E+4 9.3218620E-1 1.2297550E+4 9.1190677E-1  
1.2297750E+4 9.4573280E-1 1.2297750E+4 9.3787501E-1 1.2297750E+4 9.2468225E-1  
1.2297950E+4 9.4760802E-1 1.2297950E+4 9.4505675E-1 1.2297950E+4 9.2179000E-1  
1.2298140E+4 9.5072760E-1 1.2298140E+4 9.5406575E-1 1.2298140E+4 9.2489000E-1  
1.2298320E+4 9.5485263E-1 1.2298320E+4 9.5886567E-1 1.2298320E+4 9.3513997E-1  
1.2298530E+4 9.5762352E-1 1.2298530E+4 9.6046663E-1 1.2298530E+4 9.4145000E-1  
1.2298740E+4 9.5973769E-1 1.2298740E+4 9.6528541E-1 1.2298740E+4 9.4070000E-1  
1.2298950E+4 9.5711255E-1 1.2298950E+4 9.7211804E-1 1.2298950E+4 9.4361512E-1  
1.2299160E+4 9.6155826E-1 1.2299160E+4 9.6916822E-1 1.2299160E+4 9.5206399E-1  
1.2299370E+4 9.6423387E-1 1.2299370E+4 9.7559001E-1 1.2299370E+4 9.5581218E-1  
1.2299560E+4 9.6866143E-1 1.2299560E+4 9.7638856E-1 1.2299560E+4 9.6111451E-1  
1.2299760E+4 9.7221086E-1 1.2299760E+4 9.7455452E-1 1.2299760E+4 9.6215398E-1  
1.2299950E+4 9.7159546E-1 1.2299950E+4 9.8343180E-1 1.2299950E+4 9.6823286E-1

1.2300140E+4 9.7465995E-1	1.2300140E+4 9.8334425E-1	1.2300140E+4 9.7223311E-1
1.2300350E+4 9.8117599E-1	1.2300350E+4 9.8405122E-1	1.2300350E+4 9.7094315E-1
1.2300570E+4 9.8283152E-1	1.2300570E+4 9.8405405E-1	1.2300570E+4 9.7857028E-1
1.2300780E+4 9.8399209E-1	1.2300780E+4 9.8938571E-1	1.2300780E+4 9.8409860E-1
1.2300990E+4 9.8603614E-1	1.2300990E+4 9.8835622E-1	1.2300990E+4 9.8897000E-1
1.2301180E+4 9.8771672E-1	1.2301180E+4 9.8742337E-1	1.2301180E+4 9.9008566E-1
1.2301370E+4 9.8981399E-1	1.2301370E+4 9.8585799E-1	1.2301370E+4 9.9304574E-1
1.2301550E+4 9.9333971E-1	1.2301550E+4 9.8902900E-1	1.2301550E+4 9.9789077E-1
1.2301750E+4 9.9549336E-1	1.2301750E+4 9.8812145E-1	1.2301750E+4 9.9760652E-1
1.2301950E+4 9.9523734E-1	1.2301950E+4 9.8990375E-1	1.2301950E+4 1.0010000E+0
1.2302150E+4 9.9971851E-1	1.2302150E+4 9.9468761E-1	1.2302150E+4 1.0073000E+0
1.2302350E+4 1.0026209E+0	1.2302350E+4 9.9708883E-1	1.2302350E+4 1.0103856E+0
1.2302540E+4 1.0035283E+0	1.2302540E+4 1.0008842E+0	1.2302540E+4 1.0120215E+0
1.2302730E+4 1.0059901E+0	1.2302730E+4 9.9670305E-1	1.2302730E+4 1.0142495E+0
1.2302910E+4 1.0039774E+0	1.2302910E+4 9.9972035E-1	1.2302910E+4 1.0136000E+0
1.2303080E+4 1.0088745E+0	1.2303080E+4 1.0022264E+0	1.2303080E+4 1.0125128E+0
1.2303250E+4 1.0115068E+0	1.2303250E+4 1.0022797E+0	1.2303250E+4 1.0126746E+0
1.2303430E+4 1.0121992E+0	1.2303430E+4 1.0073886E+0	1.2303430E+4 1.0164916E+0
1.2303630E+4 1.0151507E+0	1.2303630E+4 1.0071802E+0	1.2303630E+4 1.0191752E+0
1.2303820E+4 1.0177133E+0	1.2303820E+4 1.0080335E+0	1.2303820E+4 1.0171295E+0
1.2304020E+4 1.0185826E+0	1.2304020E+4 1.0093944E+0	1.2304020E+4 1.0197824E+0
1.2304200E+4 1.0173890E+0	1.2304200E+4 1.0072414E+0	1.2304200E+4 1.0249642E+0
1.2304390E+4 1.0222801E+0	1.2304390E+4 1.0098787E+0	1.2304390E+4 1.0268896E+0
1.2304570E+4 1.0220240E+0	1.2304570E+4 1.0139279E+0	1.2304570E+4 1.0270070E+0
1.2304750E+4 1.0252158E+0	1.2304750E+4 1.0143620E+0	1.2304750E+4 1.0253572E+0
1.2304940E+4 1.0261492E+0	1.2304940E+4 1.0110019E+0	1.2304940E+4 1.0273391E+0
1.2305140E+4 1.0251434E+0	1.2305140E+4 1.0150056E+0	1.2305140E+4 1.0278147E+0
1.2305350E+4 1.0248659E+0	1.2305350E+4 1.0144572E+0	1.2305350E+4 1.0244713E+0
1.2305550E+4 1.0300195E+0	1.2305550E+4 1.0130839E+0	1.2305550E+4 1.0286334E+0
1.2305750E+4 1.0298989E+0	1.2305750E+4 1.0142141E+0	1.2305750E+4 1.0311018E+0
1.2305950E+4 1.0304271E+0	1.2305950E+4 1.0239758E+0	1.2305950E+4 1.0317987E+0
1.2306130E+4 1.0318510E+0	1.2306130E+4 1.0147197E+0	1.2306130E+4 1.0310828E+0
1.2306320E+4 1.0343843E+0	1.2306320E+4 1.0164740E+0	1.2306320E+4 1.0352533E+0
1.2306500E+4 1.0342949E+0	1.2306500E+4 1.0162838E+0	1.2306500E+4 1.0395143E+0
1.2306700E+4 1.0360597E+0	1.2306700E+4 1.0171727E+0	1.2306700E+4 1.0334201E+0
1.2306900E+4 1.0360930E+0	1.2306900E+4 1.0218701E+0	1.2306900E+4 1.0369646E+0
1.2307100E+4 1.0358349E+0	1.2307100E+4 1.0149353E+0	1.2307100E+4 1.0347151E+0
1.2307290E+4 1.0380508E+0	1.2307290E+4 1.0139719E+0	1.2307290E+4 1.0362896E+0
1.2307490E+4 1.0396409E+0	1.2307490E+4 1.0217297E+0	1.2307490E+4 1.0398347E+0
1.2307660E+4 1.0371964E+0	1.2307660E+4 1.0161762E+0	1.2307660E+4 1.0371885E+0
1.2307840E+4 1.0358256E+0	1.2307840E+4 1.0169227E+0	1.2307840E+4 1.0376593E+0
1.2308020E+4 1.0371378E+0	1.2308020E+4 1.0186849E+0	1.2308020E+4 1.0380272E+0
1.2308230E+4 1.0423680E+0	1.2308230E+4 1.0216425E+0	1.2308230E+4 1.0428605E+0
1.2308440E+4 1.0433320E+0	1.2308440E+4 1.0230242E+0	1.2308440E+4 1.0455590E+0
1.2308650E+4 1.0426204E+0	1.2308650E+4 1.0225856E+0	1.2308650E+4 1.0411850E+0
1.2308860E+4 1.0448831E+0	1.2308860E+4 1.0173483E+0	1.2308860E+4 1.0393394E+0
1.2309060E+4 1.0465104E+0	1.2309060E+4 1.0244278E+0	1.2309060E+4 1.0412525E+0
1.2309260E+4 1.0446422E+0	1.2309260E+4 1.0236631E+0	1.2309260E+4 1.0462416E+0
1.2309450E+4 1.0448996E+0	1.2309450E+4 1.0248184E+0	1.2309450E+4 1.0439378E+0
1.2309650E+4 1.0420314E+0	1.2309650E+4 1.0271124E+0	1.2309650E+4 1.0447127E+0
1.2309860E+4 1.0436862E+0	1.2309860E+4 1.0305543E+0	1.2309860E+4 1.0461940E+0
1.2310070E+4 1.0445103E+0	1.2310070E+4 1.0314890E+0	1.2310070E+4 1.0433911E+0

1.2310280E+4	1.0474578E+0	1.2310280E+4	1.0305784E+0	1.2310280E+4	1.0449863E+0
1.2310490E+4	1.0508704E+0	1.2310490E+4	1.0348108E+0	1.2310490E+4	1.0489718E+0
1.2310700E+4	1.0497862E+0	1.2310700E+4	1.0371407E+0	1.2310700E+4	1.0430435E+0
1.2310900E+4	1.0494021E+0	1.2310900E+4	1.0381253E+0	1.2310900E+4	1.0511055E+0
1.2311090E+4	1.0498739E+0	1.2311090E+4	1.0392181E+0	1.2311090E+4	1.0463433E+0
1.2311280E+4	1.0494237E+0	1.2311280E+4	1.0376144E+0	1.2311280E+4	1.0446051E+0
1.2311470E+4	1.0503517E+0	1.2311470E+4	1.0460444E+0	1.2311470E+4	1.0414021E+0
1.2311680E+4	1.0530550E+0	1.2311680E+4	1.0426383E+0	1.2311680E+4	1.0349695E+0
1.2311890E+4	1.0467328E+0	1.2311890E+4	1.0435935E+0	1.2311890E+4	1.0415138E+0
1.2312100E+4	1.0460441E+0	1.2312100E+4	1.0430531E+0	1.2312100E+4	1.0468523E+0
1.2312310E+4	1.0506282E+0	1.2312310E+4	1.0442213E+0	1.2312310E+4	1.0423500E+0
1.2312500E+4	1.0512844E+0	1.2312500E+4	1.0478462E+0	1.2312500E+4	1.0378278E+0
1.2312700E+4	1.0513789E+0	1.2312700E+4	1.0561148E+0	1.2312700E+4	1.0413643E+0
1.2312890E+4	1.0536849E+0	1.2312890E+4	1.0540197E+0	1.2312890E+4	1.0446000E+0
1.2313080E+4	1.0558731E+0	1.2313080E+4	1.0490804E+0	1.2313080E+4	1.0464698E+0
1.2313290E+4	1.0515466E+0	1.2313290E+4	1.0506445E+0	1.2313290E+4	1.0434947E+0
1.2313510E+4	1.0528160E+0	1.2313510E+4	1.0530550E+0	1.2313510E+4	1.0457626E+0
1.2313720E+4	1.0546896E+0	1.2313720E+4	1.0574804E+0	1.2313720E+4	1.0447988E+0
1.2313930E+4	1.0563143E+0	1.2313930E+4	1.0566201E+0	1.2313930E+4	1.0423687E+0
1.2314140E+4	1.0579040E+0	1.2314140E+4	1.0518579E+0	1.2314140E+4	1.0391071E+0
1.2314340E+4	1.0607170E+0	1.2314340E+4	1.0519228E+0	1.2314340E+4	1.0467343E+0
1.2314530E+4	1.0615592E+0	1.2314530E+4	1.0560129E+0	1.2314530E+4	1.0411724E+0
1.2314720E+4	1.0585104E+0	1.2314720E+4	1.0572579E+0	1.2314720E+4	1.0387873E+0
1.2314910E+4	1.0600473E+0	1.2314910E+4	1.0495047E+0	1.2314910E+4	1.0390835E+0
1.2315120E+4	1.0618763E+0	1.2315120E+4	1.0479692E+0	1.2315120E+4	1.0377089E+0
1.2315330E+4	1.0607462E+0	1.2315330E+4	1.0543151E+0	1.2315330E+4	1.0415356E+0
1.2315530E+4	1.0615012E+0	1.2315530E+4	1.0616423E+0	1.2315530E+4	1.0375544E+0
1.2315720E+4	1.0616607E+0	1.2315720E+4	1.0577774E+0	1.2315720E+4	1.0344434E+0
1.2315910E+4	1.0642399E+0	1.2315910E+4	1.0544283E+0	1.2315910E+4	1.0411324E+0
1.2316100E+4	1.0641907E+0	1.2316100E+4	1.0570410E+0	1.2316100E+4	1.0403623E+0
1.2316270E+4	1.0623761E+0	1.2316270E+4	1.0539008E+0	1.2316270E+4	1.0362398E+0
1.2316450E+4	1.0618253E+0	1.2316450E+4	1.0532559E+0	1.2316450E+4	1.0415174E+0
1.2316640E+4	1.0622933E+0	1.2316640E+4	1.0555688E+0	1.2316640E+4	1.0407269E+0
1.2316840E+4	1.0610808E+0	1.2316840E+4	1.0555056E+0	1.2316840E+4	1.0453852E+0
1.2317040E+4	1.0617096E+0	1.2317040E+4	1.0506512E+0	1.2317040E+4	1.0431133E+0
1.2317240E+4	1.0667116E+0	1.2317240E+4	1.0494443E+0	1.2317240E+4	1.0410821E+0
1.2317430E+4	1.0695483E+0	1.2317430E+4	1.0529690E+0	1.2317430E+4	1.0383844E+0
1.2317620E+4	1.0679432E+0	1.2317620E+4	1.0566515E+0	1.2317620E+4	1.0371558E+0
1.2317800E+4	1.0669582E+0	1.2317800E+4	1.0456776E+0	1.2317800E+4	1.0392378E+0
1.2317990E+4	1.0674364E+0	1.2317990E+4	1.0456059E+0	1.2317990E+4	1.0371479E+0
1.2318180E+4	1.0637793E+0	1.2318180E+4	1.0418195E+0	1.2318180E+4	1.0357610E+0
1.2318400E+4	1.0664160E+0	1.2318400E+4	1.0475700E+0	1.2318400E+4	1.0364373E+0
1.2318620E+4	1.0695971E+0	1.2318620E+4	1.0492612E+0	1.2318620E+4	1.0356487E+0
1.2318820E+4	1.0679346E+0	1.2318820E+4	1.0451665E+0	1.2318820E+4	1.0302144E+0
1.2319030E+4	1.0675859E+0	1.2319030E+4	1.0453273E+0	1.2319030E+4	1.0372852E+0
1.2319220E+4	1.0691072E+0	1.2319220E+4	1.0397819E+0	1.2319220E+4	1.0408177E+0
1.2319420E+4	1.0692844E+0	1.2319420E+4	1.0380575E+0	1.2319420E+4	1.0381444E+0
1.2319600E+4	1.0691400E+0	1.2319600E+4	1.0404703E+0	1.2319600E+4	1.0392344E+0
1.2319780E+4	1.0691007E+0	1.2319780E+4	1.0369450E+0	1.2319780E+4	1.0362008E+0
1.2319990E+4	1.0690793E+0	1.2319990E+4	1.0339676E+0	1.2319990E+4	1.0356805E+0
1.2320210E+4	1.0678043E+0	1.2320210E+4	1.0331803E+0	1.2320210E+4	1.0377758E+0
1.2320420E+4	1.0639516E+0	1.2320420E+4	1.0369733E+0	1.2320420E+4	1.0351020E+0

1.2320620E+4	1.0666618E+0	1.2320620E+4	1.0335904E+0	1.2320620E+4	1.0380896E+0
1.2320810E+4	1.0687680E+0	1.2320810E+4	1.0338164E+0	1.2320810E+4	1.0418991E+0
1.2321000E+4	1.0648999E+0	1.2321000E+4	1.0356288E+0	1.2321000E+4	1.0395065E+0
1.2321180E+4	1.0668529E+0	1.2321180E+4	1.0293119E+0	1.2321180E+4	1.0392745E+0
1.2321370E+4	1.0710289E+0	1.2321370E+4	1.0267337E+0	1.2321370E+4	1.0387041E+0
1.2321580E+4	1.0681703E+0	1.2321580E+4	1.0283789E+0	1.2321580E+4	1.0342671E+0
1.2321800E+4	1.0663667E+0	1.2321800E+4	1.0275320E+0	1.2321800E+4	1.0362866E+0
1.2322010E+4	1.0658738E+0	1.2322010E+4	1.0287432E+0	1.2322010E+4	1.0326244E+0
1.2322220E+4	1.0662449E+0	1.2322220E+4	1.0311816E+0	1.2322220E+4	1.0365790E+0
1.2322430E+4	1.0638735E+0	1.2322430E+4	1.0277173E+0	1.2322430E+4	1.0354406E+0
1.2322640E+4	1.0655314E+0	1.2322640E+4	1.0219085E+0	1.2322640E+4	1.0374566E+0
1.2322850E+4	1.0698874E+0	1.2322850E+4	1.0231418E+0	1.2322850E+4	1.0373120E+0
1.2323050E+4	1.0678272E+0	1.2323050E+4	1.0200901E+0	1.2323050E+4	1.0370291E+0
1.2323260E+4	1.0662157E+0	1.2323260E+4	1.0191973E+0	1.2323260E+4	1.0359017E+0
1.2323490E+4	1.0596459E+0	1.2323490E+4	1.0245414E+0	1.2323490E+4	1.0344367E+0
1.2323720E+4	1.0616857E+0	1.2323720E+4	1.0185088E+0	1.2323720E+4	1.0367904E+0
1.2323930E+4	1.0710397E+0	1.2323930E+4	1.0181202E+0	1.2323930E+4	1.0365249E+0
1.2324150E+4	1.0673969E+0	1.2324150E+4	1.0191377E+0	1.2324150E+4	1.0339589E+0
1.2324360E+4	1.0645113E+0	1.2324360E+4	1.0206506E+0	1.2324360E+4	1.0366177E+0
1.2324550E+4	1.0653797E+0	1.2324550E+4	1.0185608E+0	1.2324550E+4	1.0298645E+0
1.2324750E+4	1.0631543E+0	1.2324750E+4	1.0136833E+0	1.2324750E+4	1.0242024E+0
1.2324940E+4	1.0621019E+0	1.2324940E+4	1.0185235E+0	1.2324940E+4	1.0293208E+0
1.2325160E+4	1.0623446E+0	1.2325160E+4	1.0214629E+0	1.2325160E+4	1.0306321E+0
1.2325370E+4	1.0599238E+0	1.2325370E+4	1.0176225E+0	1.2325370E+4	1.0320765E+0
1.2325590E+4	1.0644922E+0	1.2325590E+4	1.0187444E+0	1.2325590E+4	1.0251536E+0
1.2325800E+4	1.0676721E+0	1.2325800E+4	1.0088840E+0	1.2325800E+4	1.0241448E+0
1.2326010E+4	1.0627356E+0	1.2326010E+4	1.0159751E+0	1.2326010E+4	1.0289202E+0
1.2326210E+4	1.0633817E+0	1.2326210E+4	1.0091721E+0	1.2326210E+4	1.0317731E+0
1.2326410E+4	1.0637625E+0	1.2326410E+4	1.0083284E+0	1.2326410E+4	1.0262000E+0
1.2326610E+4	1.0618692E+0	1.2326610E+4	1.0057749E+0	1.2326610E+4	1.0214000E+0
1.2326820E+4	1.0617931E+0	1.2326820E+4	1.0040685E+0	1.2326820E+4	1.0261000E+0
1.2327040E+4	1.0568344E+0	1.2327040E+4	1.0022128E+0	1.2327040E+4	1.0208057E+0
1.2327260E+4	1.0550885E+0	1.2327260E+4	1.0053046E+0	1.2327260E+4	1.0231981E+0
1.2327480E+4	1.0621450E+0	1.2327480E+4	1.0061567E+0	1.2327480E+4	1.0235145E+0
1.2327700E+4	1.0601505E+0	1.2327700E+4	1.0040802E+0	1.2327700E+4	1.0214099E+0
1.2327890E+4	1.0545206E+0	1.2327890E+4	9.9953916E-1	1.2327890E+4	1.0160507E+0
1.2328080E+4	1.0578064E+0	1.2328080E+4	9.9573706E-1	1.2328080E+4	1.0180019E+0
1.2328270E+4	1.0572409E+0	1.2328270E+4	9.9341381E-1	1.2328270E+4	1.0179519E+0
1.2328460E+4	1.0547056E+0	1.2328460E+4	9.8951157E-1	1.2328460E+4	1.0122617E+0
1.2328670E+4	1.0525424E+0	1.2328670E+4	9.8713033E-1	1.2328670E+4	1.0153665E+0
1.2328870E+4	1.0537951E+0	1.2328870E+4	9.8760298E-1	1.2328870E+4	1.0189490E+0
1.2329080E+4	1.0534322E+0	1.2329080E+4	9.8750868E-1	1.2329080E+4	1.0180152E+0
1.2329280E+4	1.0509524E+0	1.2329280E+4	9.9103277E-1	1.2329280E+4	1.0138125E+0
1.2329470E+4	1.0510582E+0	1.2329470E+4	9.8213334E-1	1.2329470E+4	1.0088827E+0
1.2329650E+4	1.0524824E+0	1.2329650E+4	9.8258262E-1	1.2329650E+4	1.0111260E+0
1.2329830E+4	1.0519860E+0	1.2329830E+4	9.8573670E-1	1.2329830E+4	1.0098926E+0
1.2330010E+4	1.0493394E+0	1.2330010E+4	9.7972610E-1	1.2330010E+4	1.0068915E+0
1.2330210E+4	1.0522556E+0	1.2330210E+4	9.7619057E-1	1.2330210E+4	1.0060684E+0
1.2330410E+4	1.0453296E+0	1.2330410E+4	9.7819850E-1	1.2330410E+4	1.0073400E+0
1.2330610E+4	1.0427648E+0	1.2330610E+4	9.7967874E-1	1.2330610E+4	1.0033535E+0
1.2330820E+4	1.0482837E+0	1.2330820E+4	9.6959633E-1	1.2330820E+4	9.9679066E-1
1.2331010E+4	1.0458791E+0	1.2331010E+4	9.6456819E-1	1.2331010E+4	1.0031174E+0

1.2331200E+4 1.0463970E+0	1.2331200E+4 9.6815594E-1	1.2331200E+4 9.9770444E-1
1.2331380E+4 1.0459817E+0	1.2331380E+4 9.7253273E-1	1.2331380E+4 9.9789165E-1
1.2331560E+4 1.0426518E+0	1.2331560E+4 9.6394753E-1	1.2331560E+4 9.9270761E-1
1.2331780E+4 1.0445849E+0	1.2331780E+4 9.6617520E-1	1.2331780E+4 9.9669584E-1
1.2331990E+4 1.0404690E+0	1.2331990E+4 9.6566328E-1	1.2331990E+4 9.9164235E-1
1.2332200E+4 1.0401433E+0	1.2332200E+4 9.6066309E-1	1.2332200E+4 9.9442986E-1
1.2332400E+4 1.0418877E+0	1.2332400E+4 9.6338980E-1	1.2332400E+4 1.0018139E+0
1.2332600E+4 1.0404342E+0	1.2332600E+4 9.6514449E-1	1.2332600E+4 9.9370838E-1
1.2332800E+4 1.0422684E+0	1.2332800E+4 9.6129554E-1	1.2332800E+4 9.9280053E-1
1.2332990E+4 1.0387904E+0	1.2332990E+4 9.6668339E-1	1.2332990E+4 9.9132158E-1
1.2333170E+4 1.0334776E+0	1.2333170E+4 9.6419245E-1	1.2333170E+4 9.9201586E-1
1.2333360E+4 1.0360898E+0	1.2333360E+4 9.5693053E-1	1.2333360E+4 9.9110587E-1
1.2333560E+4 1.0316185E+0	1.2333560E+4 9.5599993E-1	1.2333560E+4 9.8952133E-1
1.2333760E+4 1.0281000E+0	1.2333760E+4 9.5615044E-1	1.2333760E+4 9.8464552E-1
1.2333970E+4 1.0292859E+0	1.2333970E+4 9.5871017E-1	1.2333970E+4 9.8484853E-1
1.2334160E+4 1.0312323E+0	1.2334160E+4 9.6165535E-1	1.2334160E+4 9.8734545E-1
1.2334350E+4 1.0295171E+0	1.2334350E+4 9.5671875E-1	1.2334350E+4 9.8541781E-1
1.2334530E+4 1.0263039E+0	1.2334530E+4 9.5740771E-1	1.2334530E+4 9.8386684E-1
1.2334710E+4 1.0300096E+0	1.2334710E+4 9.5898064E-1	1.2334710E+4 9.8303982E-1
1.2334900E+4 1.0328346E+0	1.2334900E+4 9.5254139E-1	1.2334900E+4 9.8240783E-1
1.2335110E+4 1.0279153E+0	1.2335110E+4 9.5206686E-1	1.2335110E+4 9.8286560E-1
1.2335320E+4 1.0226878E+0	1.2335320E+4 9.5017176E-1	1.2335320E+4 9.7741315E-1
1.2335540E+4 1.0234923E+0	1.2335540E+4 9.5350957E-1	1.2335540E+4 9.7708353E-1
1.2335750E+4 1.0189758E+0	1.2335750E+4 9.5656629E-1	1.2335750E+4 9.7813898E-1
1.2335960E+4 1.0219900E+0	1.2335960E+4 9.5485214E-1	1.2335960E+4 9.7662036E-1
1.2336160E+4 1.0227896E+0	1.2336160E+4 9.5155756E-1	1.2336160E+4 9.7461288E-1
1.2336360E+4 1.0190699E+0	1.2336360E+4 9.5027279E-1	1.2336360E+4 9.7547278E-1
1.2336560E+4 1.0190667E+0	1.2336560E+4 9.5251828E-1	1.2336560E+4 9.7330385E-1
1.2336760E+4 1.0164364E+0	1.2336760E+4 9.5383929E-1	1.2336760E+4 9.7750951E-1
1.2336980E+4 1.0199830E+0	1.2336980E+4 9.5527129E-1	1.2336980E+4 9.7088340E-1
1.2337200E+4 1.0170068E+0	1.2337200E+4 9.5752504E-1	1.2337200E+4 9.6826890E-1
1.2337410E+4 1.0124353E+0	1.2337410E+4 9.5383760E-1	1.2337410E+4 9.7480853E-1
1.2337620E+4 1.0166648E+0	1.2337620E+4 9.5449618E-1	1.2337620E+4 9.7193150E-1
1.2337810E+4 1.0184881E+0	1.2337810E+4 9.5016715E-1	1.2337810E+4 9.6654716E-1
1.2338010E+4 1.0162297E+0	1.2338010E+4 9.5150512E-1	1.2338010E+4 9.6824033E-1
1.2338190E+4 1.0107111E+0	1.2338190E+4 9.5528346E-1	1.2338190E+4 9.6907555E-1
1.2338390E+4 1.0071044E+0	1.2338390E+4 9.5211506E-1	1.2338390E+4 9.6763702E-1
1.2338590E+4 1.0094899E+0	1.2338590E+4 9.5273865E-1	1.2338590E+4 9.6913922E-1
1.2338800E+4 1.0105643E+0	1.2338800E+4 9.5212634E-1	1.2338800E+4 9.6353018E-1
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1.2339620E+4 1.0020944E+0	1.2339620E+4 9.5117372E-1	1.2339620E+4 9.6396320E-1
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1.2340210E+4 1.0033874E+0	1.2340210E+4 9.4773825E-1	1.2340210E+4 9.6217938E-1
1.2340410E+4 9.9868131E-1	1.2340410E+4 9.5314715E-1	1.2340410E+4 9.6417094E-1
1.2340630E+4 9.9725508E-1	1.2340630E+4 9.5201657E-1	1.2340630E+4 9.5529033E-1
1.2340840E+4 9.9713076E-1	1.2340840E+4 9.5586582E-1	1.2340840E+4 9.6958003E-1
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1.2352400E+4 9.9179616E-1	1.2352400E+4 9.9985368E-1	1.2352400E+4 9.8146296E-1
1.2352620E+4 9.9286903E-1	1.2352620E+4 9.9018239E-1	1.2352620E+4 9.8551986E-1
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1.2353230E+4 9.9774109E-1	1.2353230E+4 9.9217774E-1	1.2353230E+4 9.8965621E-1
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1.2353620E+4 9.9376508E-1	1.2353620E+4 9.9378273E-1	1.2353620E+4 9.8877000E-1
1.2353840E+4 9.9356052E-1	1.2353840E+4 9.9487605E-1	1.2353840E+4 9.9303808E-1
1.2354060E+4 9.9334028E-1	1.2354060E+4 1.0031790E+0	1.2354060E+4 9.9956810E-1
1.2354290E+4 9.9545288E-1	1.2354290E+4 9.9436432E-1	1.2354290E+4 9.9416747E-1
1.2354500E+4 9.9194765E-1	1.2354500E+4 9.9628410E-1	1.2354500E+4 9.9203543E-1
1.2354690E+4 9.9359703E-1	1.2354690E+4 9.9880095E-1	1.2354690E+4 9.9695403E-1
1.2354890E+4 1.0005708E+0	1.2354890E+4 9.9821959E-1	1.2354890E+4 9.9608189E-1
1.2355070E+4 9.9951233E-1	1.2355070E+4 9.9978903E-1	1.2355070E+4 1.0001744E+0
1.2355270E+4 1.0031227E+0	1.2355270E+4 1.0010999E+0	1.2355270E+4 9.9351000E-1
1.2355470E+4 1.0008590E+0	1.2355470E+4 9.9884947E-1	1.2355470E+4 9.9132253E-1
1.2355680E+4 1.0010899E+0	1.2355680E+4 9.9839113E-1	1.2355680E+4 9.9661329E-1
1.2355890E+4 9.9862540E-1	1.2355890E+4 1.0027256E+0	1.2355890E+4 1.0025689E+0
1.2356080E+4 1.0004276E+0	1.2356080E+4 1.0034884E+0	1.2356080E+4 1.0042133E+0
1.2356280E+4 9.9785124E-1	1.2356280E+4 1.0013211E+0	1.2356280E+4 1.0002715E+0
1.2356470E+4 1.0015172E+0	1.2356470E+4 1.0060071E+0	1.2356470E+4 9.9287412E-1

### Hg(SR)<sub>3</sub>

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1.2258980E+4 2.9279000E-4  
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1.2259410E+4 1.1997821E-5  
1.2259620E+4 5.9222839E-5  
1.2259820E+4 6.7677286E-5  
1.2260020E+4 6.6575450E-5  
1.2260210E+4 1.1525363E-4  
1.2260400E+4 1.3358196E-4  
1.2260590E+4 8.2602259E-5  
1.2260800E+4 9.0672745E-5  
1.2261020E+4 1.0395420E-4  
1.2261230E+4 1.4588806E-4  
1.2261440E+4 1.2882540E-4  
1.2261630E+4 9.1491050E-5  
1.2261830E+4 1.2204189E-4  
1.2262010E+4 1.4765163E-4  
1.2262190E+4 1.5182299E-4  
1.2262390E+4 1.6792420E-4  
1.2262600E+4 1.7252637E-4  
1.2262800E+4 1.8368653E-4  
1.2263000E+4 1.3988034E-4  
1.2263190E+4 2.3067434E-4  
1.2263370E+4 2.0058951E-4  
1.2263540E+4 1.8209966E-4  
1.2263710E+4 2.3057713E-4

### Hg(PC2)

1.2258820E+4 8.4837000E-5  
1.2258840E+4 9.3373000E-5  
1.2258980E+4 2.1279000E-4  
1.2259200E+4 0.0000000E+0  
1.2259410E+4 2.0630000E-4  
1.2259620E+4 1.9205000E-4  
1.2259820E+4 1.1430000E-4  
1.2260020E+4 1.8970000E-4  
1.2260210E+4 1.8316000E-4  
1.2260400E+4 2.2529000E-4  
1.2260590E+4 1.7395000E-4  
1.2260800E+4 2.3655000E-4  
1.2261020E+4 1.6034000E-4  
1.2261230E+4 2.8086000E-4  
1.2261440E+4 2.1084000E-4  
1.2261630E+4 1.4807000E-4  
1.2261830E+4 1.5691000E-4  
1.2262010E+4 2.3473000E-4  
1.2262190E+4 1.8187000E-4  
1.2262390E+4 2.5523000E-4  
1.2262600E+4 2.9351000E-4  
1.2262800E+4 2.9599000E-4  
1.2263000E+4 3.5985000E-4  
1.2263190E+4 2.8714000E-4  
1.2263370E+4 3.2689000E-4  
1.2263540E+4 3.1989000E-4  
1.2263710E+4 3.5693000E-4

### Hg(Cys)<sub>4</sub>

1.2258820E+4 8.4297000E-5  
1.2258840E+4 9.3183000E-5  
1.2258980E+4 2.0079000E-4  
1.2259200E+4 0.0120000E+0  
1.2259410E+4 2.0030000E-4  
1.2259620E+4 1.9105000E-4  
1.2259820E+4 3.0249801E-4  
1.2260020E+4 4.8345085E-4  
1.2260210E+4 6.4392800E-4  
1.2260400E+4 5.5144199E-4  
1.2260590E+4 3.4846652E-4  
1.2260800E+4 2.1092944E-4  
1.2261020E+4 2.6751584E-4  
1.2261230E+4 5.1496760E-4  
1.2261440E+4 4.5830001E-4  
1.2261630E+4 4.0206037E-4  
1.2261830E+4 5.4299845E-4  
1.2262010E+4 5.7013522E-4  
1.2262190E+4 4.6601131E-4  
1.2262390E+4 3.5371978E-4  
1.2262600E+4 3.2252248E-4  
1.2262800E+4 3.0621712E-4  
1.2263000E+4 5.8822441E-4  
1.2263190E+4 6.5225708E-4  
1.2263370E+4 5.9527714E-4  
1.2263540E+4 3.2100332E-4  
1.2263710E+4 4.7356940E-4

1.2263890E+4	2.1395314E-4	1.2263890E+4	3.6861000E-4	1.2263890E+4	5.4628145E-4
1.2264080E+4	2.8146545E-4	1.2264080E+4	4.9558000E-4	1.2264080E+4	6.3848328E-4
1.2264270E+4	2.8748464E-4	1.2264270E+4	3.3569000E-4	1.2264270E+4	5.6974747E-4
1.2264460E+4	2.7451825E-4	1.2264460E+4	4.4153000E-4	1.2264460E+4	6.8825999E-4
1.2264660E+4	2.5519272E-4	1.2264660E+4	4.0898000E-4	1.2264660E+4	5.6947617E-4
1.2264840E+4	3.4782851E-4	1.2264840E+4	4.4075000E-4	1.2264840E+4	5.2865789E-4
1.2265020E+4	4.4411531E-4	1.2265020E+4	4.5381000E-4	1.2265020E+4	5.6592429E-4
1.2265200E+4	3.9050566E-4	1.2265200E+4	4.8053000E-4	1.2265200E+4	7.5266562E-4
1.2265390E+4	3.6605000E-4	1.2265390E+4	6.1214000E-4	1.2265390E+4	8.3380866E-4
1.2265590E+4	3.5325116E-4	1.2265590E+4	5.8583000E-4	1.2265590E+4	5.3023275E-4
1.2265790E+4	4.8592479E-4	1.2265790E+4	5.0760000E-4	1.2265790E+4	4.1238661E-4
1.2265990E+4	4.5587516E-4	1.2265990E+4	6.6583000E-4	1.2265990E+4	5.8701310E-4
1.2266190E+4	5.2448071E-4	1.2266190E+4	4.3892000E-4	1.2266190E+4	6.8289043E-4
1.2266380E+4	5.2719634E-4	1.2266380E+4	6.7310000E-4	1.2266380E+4	1.0636606E-3
1.2266560E+4	4.6980458E-4	1.2266560E+4	7.7664000E-4	1.2266560E+4	1.0089320E-3
1.2266740E+4	5.6841650E-4	1.2266740E+4	6.4894000E-4	1.2266740E+4	1.0003442E-3
1.2266920E+4	6.4595055E-4	1.2266920E+4	8.4145000E-4	1.2266920E+4	6.1336701E-4
1.2267110E+4	6.5701813E-4	1.2267110E+4	8.7882000E-4	1.2267110E+4	8.9072625E-4
1.2267310E+4	6.3865945E-4	1.2267310E+4	9.0564000E-4	1.2267310E+4	8.0120956E-4
1.2267500E+4	7.1350817E-4	1.2267500E+4	1.0451000E-3	1.2267500E+4	9.4538839E-4
1.2267700E+4	7.7242000E-4	1.2267700E+4	1.0886000E-3	1.2267700E+4	1.0188520E-3
1.2267880E+4	8.6200000E-4	1.2267880E+4	1.1931000E-3	1.2267880E+4	1.0902495E-3
1.2268060E+4	9.0840636E-4	1.2268060E+4	1.0968000E-3	1.2268060E+4	9.9549735E-4
1.2268230E+4	9.7162000E-4	1.2268230E+4	1.3141000E-3	1.2268230E+4	1.0584871E-3
1.2268410E+4	1.0759484E-3	1.2268410E+4	1.2474000E-3	1.2268410E+4	1.0448991E-3
1.2268590E+4	1.1270969E-3	1.2268590E+4	1.1071000E-3	1.2268590E+4	1.1200644E-3
1.2268790E+4	1.1111263E-3	1.2268790E+4	1.3196000E-3	1.2268790E+4	1.4163113E-3
1.2268990E+4	1.1265882E-3	1.2268990E+4	1.5287000E-3	1.2268990E+4	1.5825896E-3
1.2269200E+4	1.2677001E-3	1.2269200E+4	1.4578000E-3	1.2269200E+4	1.3435966E-3
1.2269400E+4	1.5486924E-3	1.2269400E+4	1.7157000E-3	1.2269400E+4	1.7443027E-3
1.2269590E+4	1.4648795E-3	1.2269590E+4	1.9391000E-3	1.2269590E+4	1.7702457E-3
1.2269770E+4	1.5662890E-3	1.2269770E+4	2.0446000E-3	1.2269770E+4	1.8309415E-3
1.2269960E+4	1.7802801E-3	1.2269960E+4	2.1744000E-3	1.2269960E+4	2.0100826E-3
1.2270150E+4	1.8852198E-3	1.2270150E+4	2.3027000E-3	1.2270150E+4	2.1909000E-3
1.2270370E+4	2.0697521E-3	1.2270370E+4	2.4467000E-3	1.2270370E+4	2.5283671E-3
1.2270580E+4	2.3304166E-3	1.2270580E+4	2.6940000E-3	1.2270580E+4	2.4678010E-3
1.2270800E+4	2.4480428E-3	1.2270800E+4	2.9041000E-3	1.2270800E+4	2.5066277E-3
1.2271010E+4	2.5679913E-3	1.2271010E+4	3.2195000E-3	1.2271010E+4	2.8483846E-3
1.2271220E+4	2.8495651E-3	1.2271220E+4	3.4585000E-3	1.2271220E+4	3.1541495E-3
1.2271410E+4	3.1473080E-3	1.2271410E+4	3.5979000E-3	1.2271410E+4	3.4942036E-3
1.2271590E+4	3.4140065E-3	1.2271590E+4	4.0200000E-3	1.2271590E+4	3.9023273E-3
1.2271780E+4	3.7124040E-3	1.2271780E+4	4.5185000E-3	1.2271780E+4	4.0073860E-3
1.2272000E+4	4.1329342E-3	1.2272000E+4	5.0533000E-3	1.2272000E+4	4.1923766E-3
1.2272210E+4	4.6141591E-3	1.2272210E+4	5.6116000E-3	1.2272210E+4	4.7823859E-3
1.2272430E+4	5.2329215E-3	1.2272430E+4	6.1355000E-3	1.2272430E+4	5.2777921E-3
1.2272640E+4	5.7371415E-3	1.2272640E+4	6.6536000E-3	1.2272640E+4	5.6341231E-3
1.2272830E+4	6.4783122E-3	1.2272830E+4	7.5956000E-3	1.2272830E+4	6.3863334E-3
1.2273020E+4	7.1408801E-3	1.2273020E+4	8.4722000E-3	1.2273020E+4	7.1856499E-3
1.2273210E+4	7.8927578E-3	1.2273210E+4	9.6585000E-3	1.2273210E+4	8.4565095E-3
1.2273410E+4	8.9752212E-3	1.2273410E+4	1.0683000E-2	1.2273410E+4	9.2163254E-3
1.2273600E+4	1.0308180E-2	1.2273600E+4	1.2192000E-2	1.2273600E+4	1.0174375E-2
1.2273820E+4	1.1974378E-2	1.2273820E+4	1.4114000E-2	1.2273820E+4	1.2055374E-2

1.2274020E+4	1.3484866E-2	1.2274020E+4	1.6474000E-2	1.2274020E+4	1.3753465E-2
1.2274230E+4	1.5497769E-2	1.2274230E+4	1.8117000E-2	1.2274230E+4	1.5989883E-2
1.2274440E+4	1.7951403E-2	1.2274440E+4	2.1499000E-2	1.2274440E+4	1.8886610E-2
1.2274630E+4	2.0995225E-2	1.2274630E+4	2.5336000E-2	1.2274630E+4	2.0989232E-2
1.2274820E+4	2.4314095E-2	1.2274820E+4	2.9148000E-2	1.2274820E+4	2.4239710E-2
1.2275010E+4	2.8675608E-2	1.2275010E+4	3.3640000E-2	1.2275010E+4	2.8255034E-2
1.2275210E+4	3.4398596E-2	1.2275210E+4	3.9410000E-2	1.2275210E+4	3.3779379E-2
1.2275410E+4	4.1292692E-2	1.2275410E+4	4.7727000E-2	1.2275410E+4	4.0020013E-2
1.2275620E+4	5.0487140E-2	1.2275620E+4	5.8489000E-2	1.2275620E+4	4.7760555E-2
1.2275820E+4	6.1686631E-2	1.2275820E+4	7.1825000E-2	1.2275820E+4	5.6673761E-2
1.2276010E+4	7.5282912E-2	1.2276010E+4	8.6931000E-2	1.2276010E+4	6.8464662E-2
1.2276200E+4	9.1408815E-2	1.2276200E+4	1.0566000E-1	1.2276200E+4	8.0156301E-2
1.2276380E+4	1.1090761E-1	1.2276380E+4	1.2698000E-1	1.2276380E+4	9.2439631E-2
1.2276560E+4	1.3374908E-1	1.2276560E+4	1.5206000E-1	1.2276560E+4	1.0984296E-1
1.2276740E+4	1.5986185E-1	1.2276740E+4	1.8174000E-1	1.2276740E+4	1.2922036E-1
1.2276930E+4	1.8803362E-1	1.2276930E+4	2.1999000E-1	1.2276930E+4	1.5217124E-1
1.2277120E+4	2.1983117E-1	1.2277120E+4	2.6355000E-1	1.2277120E+4	1.7645940E-1
1.2277310E+4	2.5711636E-1	1.2277310E+4	3.1055000E-1	1.2277310E+4	2.0180780E-1
1.2277510E+4	2.9554609E-1	1.2277510E+4	3.6277000E-1	1.2277510E+4	2.3247743E-1
1.2277700E+4	3.2903420E-1	1.2277700E+4	4.1486000E-1	1.2277700E+4	2.6328960E-1
1.2277880E+4	3.6234680E-1	1.2277880E+4	4.6145000E-1	1.2277880E+4	2.9311429E-1
1.2278060E+4	3.9504573E-1	1.2278060E+4	5.0804000E-1	1.2278060E+4	3.2314791E-1
1.2278240E+4	4.2358539E-1	1.2278240E+4	5.5283000E-1	1.2278240E+4	3.5166105E-1
1.2278450E+4	4.5171986E-1	1.2278450E+4	5.8982000E-1	1.2278450E+4	3.8742076E-1
1.2278660E+4	4.7726085E-1	1.2278660E+4	6.2418000E-1	1.2278660E+4	4.2363599E-1
1.2278860E+4	4.9708345E-1	1.2278860E+4	6.4405000E-1	1.2278860E+4	4.5542208E-1
1.2279060E+4	5.1329837E-1	1.2279060E+4	6.5696000E-1	1.2279060E+4	4.8127785E-1
1.2279260E+4	5.2769023E-1	1.2279260E+4	6.5785000E-1	1.2279260E+4	5.0587955E-1
1.2279450E+4	5.3691673E-1	1.2279450E+4	6.4827000E-1	1.2279450E+4	5.3117017E-1
1.2279640E+4	5.4532680E-1	1.2279640E+4	6.3394000E-1	1.2279640E+4	5.5360744E-1
1.2279830E+4	5.5515059E-1	1.2279830E+4	6.1560000E-1	1.2279830E+4	5.7346406E-1
1.2280020E+4	5.6338197E-1	1.2280020E+4	5.9654000E-1	1.2280020E+4	5.9240867E-1
1.2280210E+4	5.7115528E-1	1.2280210E+4	5.7211000E-1	1.2280210E+4	6.1097686E-1
1.2280420E+4	5.8053541E-1	1.2280420E+4	5.4663000E-1	1.2280420E+4	6.2591803E-1
1.2280630E+4	5.8537129E-1	1.2280630E+4	5.2460000E-1	1.2280630E+4	6.4017442E-1
1.2280830E+4	5.9280522E-1	1.2280830E+4	5.0771000E-1	1.2280830E+4	6.5268038E-1
1.2281010E+4	5.9595516E-1	1.2281010E+4	4.9667000E-1	1.2281010E+4	6.6159779E-1
1.2281190E+4	5.9748728E-1	1.2281190E+4	4.8889000E-1	1.2281190E+4	6.6594190E-1
1.2281370E+4	6.0213738E-1	1.2281370E+4	4.8493000E-1	1.2281370E+4	6.6908217E-1
1.2281560E+4	6.0514809E-1	1.2281560E+4	4.8272000E-1	1.2281560E+4	6.7560077E-1
1.2281760E+4	6.0387653E-1	1.2281760E+4	4.8966000E-1	1.2281760E+4	6.8049824E-1
1.2281970E+4	6.0183811E-1	1.2281970E+4	4.9424000E-1	1.2281970E+4	6.8388942E-1
1.2282180E+4	6.0095772E-1	1.2282180E+4	5.0521000E-1	1.2282180E+4	6.8611906E-1
1.2282380E+4	6.0471421E-1	1.2282380E+4	5.1690000E-1	1.2282380E+4	6.9150252E-1
1.2282580E+4	6.0672995E-1	1.2282580E+4	5.3417000E-1	1.2282580E+4	6.9477803E-1
1.2282790E+4	6.0771406E-1	1.2282790E+4	5.4968000E-1	1.2282790E+4	7.0005000E-1
1.2282990E+4	6.1438131E-1	1.2282990E+4	5.6673000E-1	1.2282990E+4	7.0583530E-1
1.2283180E+4	6.1841293E-1	1.2283180E+4	5.8354000E-1	1.2283180E+4	7.1167384E-1
1.2283400E+4	6.2728954E-1	1.2283400E+4	6.0327000E-1	1.2283400E+4	7.1931088E-1
1.2283620E+4	6.4057870E-1	1.2283620E+4	6.2494000E-1	1.2283620E+4	7.2219530E-1
1.2283840E+4	6.5350746E-1	1.2283840E+4	6.4809000E-1	1.2283840E+4	7.2720345E-1
1.2284070E+4	6.6786903E-1	1.2284070E+4	6.6936000E-1	1.2284070E+4	7.3355871E-1

1.2284290E+4 6.8132387E-1	1.2284290E+4 6.9377000E-1	1.2284290E+4 7.3789561E-1
1.2284490E+4 6.9616827E-1	1.2284490E+4 7.1594000E-1	1.2284490E+4 7.3858488E-1
1.2284680E+4 7.1017519E-1	1.2284680E+4 7.3639000E-1	1.2284680E+4 7.3906555E-1
1.2284870E+4 7.2559353E-1	1.2284870E+4 7.5270000E-1	1.2284870E+4 7.3922564E-1
1.2285090E+4 7.4409970E-1	1.2285090E+4 7.7315000E-1	1.2285090E+4 7.4033053E-1
1.2285300E+4 7.5982199E-1	1.2285300E+4 7.9397000E-1	1.2285300E+4 7.4308294E-1
1.2285520E+4 7.7272109E-1	1.2285520E+4 8.1256000E-1	1.2285520E+4 7.4040405E-1
1.2285730E+4 7.8664466E-1	1.2285730E+4 8.3135000E-1	1.2285730E+4 7.3834582E-1
1.2285940E+4 7.9686073E-1	1.2285940E+4 8.4782000E-1	1.2285940E+4 7.3729909E-1
1.2286150E+4 8.0508884E-1	1.2286150E+4 8.6049000E-1	1.2286150E+4 7.3382168E-1
1.2286350E+4 8.1469774E-1	1.2286350E+4 8.7084000E-1	1.2286350E+4 7.3260974E-1
1.2286540E+4 8.1643151E-1	1.2286540E+4 8.7953000E-1	1.2286540E+4 7.3107759E-1
1.2286750E+4 8.1755369E-1	1.2286750E+4 8.8770000E-1	1.2286750E+4 7.3006512E-1
1.2286970E+4 8.2392192E-1	1.2286970E+4 8.9442000E-1	1.2286970E+4 7.3005641E-1
1.2287190E+4 8.2588742E-1	1.2287190E+4 9.0259000E-1	1.2287190E+4 7.2518666E-1
1.2287410E+4 8.2339965E-1	1.2287410E+4 9.0670000E-1	1.2287410E+4 7.2260390E-1
1.2287620E+4 8.1964365E-1	1.2287620E+4 9.0953000E-1	1.2287620E+4 7.2630468E-1
1.2287830E+4 8.1646924E-1	1.2287830E+4 9.1113000E-1	1.2287830E+4 7.2893189E-1
1.2288030E+4 8.1060669E-1	1.2288030E+4 9.1204000E-1	1.2288030E+4 7.2910348E-1
1.2288220E+4 8.0798600E-1	1.2288220E+4 9.1475000E-1	1.2288220E+4 7.3028736E-1
1.2288410E+4 8.0965375E-1	1.2288410E+4 9.2106000E-1	1.2288410E+4 7.3247274E-1
1.2288620E+4 8.0109373E-1	1.2288620E+4 9.1829000E-1	1.2288620E+4 7.3888509E-1
1.2288840E+4 7.9824744E-1	1.2288840E+4 9.2186000E-1	1.2288840E+4 7.4616003E-1
1.2289040E+4 7.9787201E-1	1.2289040E+4 9.2171000E-1	1.2289040E+4 7.4870475E-1
1.2289240E+4 7.9354652E-1	1.2289240E+4 9.1955000E-1	1.2289240E+4 7.5312754E-1
1.2289430E+4 7.9346554E-1	1.2289430E+4 9.2100000E-1	1.2289430E+4 7.5378463E-1
1.2289620E+4 7.9672049E-1	1.2289620E+4 9.2051000E-1	1.2289620E+4 7.5977372E-1
1.2289800E+4 7.9765472E-1	1.2289800E+4 9.1962000E-1	1.2289800E+4 7.6407614E-1
1.2289990E+4 7.9558158E-1	1.2289990E+4 9.1753000E-1	1.2289990E+4 7.7091023E-1
1.2290170E+4 7.9733864E-1	1.2290170E+4 9.1845000E-1	1.2290170E+4 7.7723811E-1
1.2290370E+4 7.9888964E-1	1.2290370E+4 9.1664000E-1	1.2290370E+4 7.8408880E-1
1.2290580E+4 8.0241054E-1	1.2290580E+4 9.1568000E-1	1.2290580E+4 7.8992904E-1
1.2290780E+4 8.0562627E-1	1.2290780E+4 9.1904000E-1	1.2290780E+4 7.9494765E-1
1.2290970E+4 8.0409749E-1	1.2290970E+4 9.1661000E-1	1.2290970E+4 8.0122421E-1
1.2291150E+4 8.0820062E-1	1.2291150E+4 9.1691000E-1	1.2291150E+4 8.0671705E-1
1.2291340E+4 8.1547627E-1	1.2291340E+4 9.1499000E-1	1.2291340E+4 8.1589293E-1
1.2291520E+4 8.1642970E-1	1.2291520E+4 9.1404000E-1	1.2291520E+4 8.2140807E-1
1.2291720E+4 8.2283995E-1	1.2291720E+4 9.1481000E-1	1.2291720E+4 8.2519353E-1
1.2291930E+4 8.2297801E-1	1.2291930E+4 9.1234000E-1	1.2291930E+4 8.3239965E-1
1.2292140E+4 8.2540696E-1	1.2292140E+4 9.1040000E-1	1.2292140E+4 8.3853926E-1
1.2292350E+4 8.3185480E-1	1.2292350E+4 9.1354000E-1	1.2292350E+4 8.4032512E-1
1.2292550E+4 8.3516587E-1	1.2292550E+4 9.1263000E-1	1.2292550E+4 8.4807275E-1
1.2292750E+4 8.4199555E-1	1.2292750E+4 9.1318000E-1	1.2292750E+4 8.5157206E-1
1.2292940E+4 8.4563418E-1	1.2292940E+4 9.1615000E-1	1.2292940E+4 8.5357640E-1
1.2293130E+4 8.4970743E-1	1.2293130E+4 9.1173000E-1	1.2293130E+4 8.5616000E-1
1.2293320E+4 8.5551999E-1	1.2293320E+4 9.1409000E-1	1.2293320E+4 8.5717958E-1
1.2293510E+4 8.5740277E-1	1.2293510E+4 9.1510000E-1	1.2293510E+4 8.5917288E-1
1.2293720E+4 8.5816476E-1	1.2293720E+4 9.1468000E-1	1.2293720E+4 8.5963102E-1
1.2293930E+4 8.6618044E-1	1.2293930E+4 9.1653000E-1	1.2293930E+4 8.6208316E-1
1.2294120E+4 8.7181193E-1	1.2294120E+4 9.1561000E-1	1.2294120E+4 8.6607915E-1
1.2294310E+4 8.7441298E-1	1.2294310E+4 9.2084000E-1	1.2294310E+4 8.6717082E-1
1.2294490E+4 8.7752924E-1	1.2294490E+4 9.2089000E-1	1.2294490E+4 8.6535362E-1

1.2294670E+4 8.8003009E-1	1.2294670E+4 9.2400000E-1	1.2294670E+4 8.6592323E-1
1.2294860E+4 8.8602790E-1	1.2294860E+4 9.2636000E-1	1.2294860E+4 8.7077903E-1
1.2295060E+4 8.9053934E-1	1.2295060E+4 9.2328000E-1	1.2295060E+4 8.7428135E-1
1.2295270E+4 8.9393440E-1	1.2295270E+4 9.2420000E-1	1.2295270E+4 8.7506370E-1
1.2295480E+4 8.9213631E-1	1.2295480E+4 9.2666000E-1	1.2295480E+4 8.7877661E-1
1.2295690E+4 8.9690826E-1	1.2295690E+4 9.2612000E-1	1.2295690E+4 8.7841913E-1
1.2295900E+4 8.9903071E-1	1.2295900E+4 9.3158000E-1	1.2295900E+4 8.8249000E-1
1.2296100E+4 9.0025000E-1	1.2296100E+4 9.3416000E-1	1.2296100E+4 8.8442691E-1
1.2296300E+4 9.0151850E-1	1.2296300E+4 9.3805000E-1	1.2296300E+4 8.8482804E-1
1.2296490E+4 9.0651000E-1	1.2296490E+4 9.3869000E-1	1.2296490E+4 8.9089955E-1
1.2296690E+4 9.1227230E-1	1.2296690E+4 9.3844000E-1	1.2296690E+4 8.9223631E-1
1.2296900E+4 9.1124809E-1	1.2296900E+4 9.4021000E-1	1.2296900E+4 8.9402045E-1
1.2297130E+4 9.1764352E-1	1.2297130E+4 9.4359000E-1	1.2297130E+4 9.0034091E-1
1.2297350E+4 9.1660896E-1	1.2297350E+4 9.4528000E-1	1.2297350E+4 9.0301142E-1
1.2297550E+4 9.1783840E-1	1.2297550E+4 9.4885000E-1	1.2297550E+4 9.0839280E-1
1.2297750E+4 9.1932460E-1	1.2297750E+4 9.4779000E-1	1.2297750E+4 9.1086297E-1
1.2297950E+4 9.2465000E-1	1.2297950E+4 9.5070000E-1	1.2297950E+4 9.1180575E-1
1.2298140E+4 9.2857000E-1	1.2298140E+4 9.5506000E-1	1.2298140E+4 9.1465563E-1
1.2298320E+4 9.2960061E-1	1.2298320E+4 9.5846000E-1	1.2298320E+4 9.1890899E-1
1.2298530E+4 9.3115139E-1	1.2298530E+4 9.6082000E-1	1.2298530E+4 9.2175374E-1
1.2298740E+4 9.3668844E-1	1.2298740E+4 9.6225000E-1	1.2298740E+4 9.2335532E-1
1.2298950E+4 9.3505000E-1	1.2298950E+4 9.6645000E-1	1.2298950E+4 9.3018438E-1
1.2299160E+4 9.3623000E-1	1.2299160E+4 9.7048000E-1	1.2299160E+4 9.3518060E-1
1.2299370E+4 9.4080000E-1	1.2299370E+4 9.7112000E-1	1.2299370E+4 9.3827215E-1
1.2299560E+4 9.3917212E-1	1.2299560E+4 9.7577000E-1	1.2299560E+4 9.4139492E-1
1.2299760E+4 9.4106767E-1	1.2299760E+4 9.7736000E-1	1.2299760E+4 9.4445440E-1
1.2299950E+4 9.4632731E-1	1.2299950E+4 9.8280000E-1	1.2299950E+4 9.4888056E-1
1.2300140E+4 9.4603983E-1	1.2300140E+4 9.8311000E-1	1.2300140E+4 9.5308723E-1
1.2300350E+4 9.4862853E-1	1.2300350E+4 9.8764000E-1	1.2300350E+4 9.5413929E-1
1.2300570E+4 9.5247000E-1	1.2300570E+4 9.8781000E-1	1.2300570E+4 9.5547252E-1
1.2300780E+4 9.5409457E-1	1.2300780E+4 9.9524000E-1	1.2300780E+4 9.6051826E-1
1.2300990E+4 9.5055701E-1	1.2300990E+4 9.9524000E-1	1.2300990E+4 9.6412323E-1
1.2301180E+4 9.6019971E-1	1.2301180E+4 9.9700000E-1	1.2301180E+4 9.6859532E-1
1.2301370E+4 9.6213117E-1	1.2301370E+4 1.0025000E+0	1.2301370E+4 9.7215937E-1
1.2301550E+4 9.6329572E-1	1.2301550E+4 1.0012000E+0	1.2301550E+4 9.7312080E-1
1.2301750E+4 9.6360759E-1	1.2301750E+4 1.0069000E+0	1.2301750E+4 9.7717000E-1
1.2301950E+4 9.6733107E-1	1.2301950E+4 1.0073000E+0	1.2301950E+4 9.8143000E-1
1.2302150E+4 9.7125779E-1	1.2302150E+4 1.0102000E+0	1.2302150E+4 9.8056423E-1
1.2302350E+4 9.7370000E-1	1.2302350E+4 1.0148000E+0	1.2302350E+4 9.8074483E-1
1.2302540E+4 9.7469000E-1	1.2302540E+4 1.0194000E+0	1.2302540E+4 9.8606477E-1
1.2302730E+4 9.7504127E-1	1.2302730E+4 1.0172000E+0	1.2302730E+4 9.9123353E-1
1.2302910E+4 9.7988530E-1	1.2302910E+4 1.0199000E+0	1.2302910E+4 9.9047180E-1
1.2303080E+4 9.8579609E-1	1.2303080E+4 1.0214000E+0	1.2303080E+4 9.8981845E-1
1.2303250E+4 9.8071975E-1	1.2303250E+4 1.0291000E+0	1.2303250E+4 9.9508547E-1
1.2303430E+4 9.8024950E-1	1.2303430E+4 1.0239000E+0	1.2303430E+4 1.0006457E+0
1.2303630E+4 9.8250392E-1	1.2303630E+4 1.0272000E+0	1.2303630E+4 1.0003832E+0
1.2303820E+4 9.8536066E-1	1.2303820E+4 1.0294000E+0	1.2303820E+4 1.0010976E+0
1.2304020E+4 9.9146717E-1	1.2304020E+4 1.0334000E+0	1.2304020E+4 1.0056154E+0
1.2304200E+4 9.8695000E-1	1.2304200E+4 1.0305000E+0	1.2304200E+4 1.0081431E+0
1.2304390E+4 9.9253684E-1	1.2304390E+4 1.0368000E+0	1.2304390E+4 1.0101041E+0
1.2304570E+4 9.9661408E-1	1.2304570E+4 1.0376000E+0	1.2304570E+4 1.0129935E+0
1.2304750E+4 9.9413851E-1	1.2304750E+4 1.0390000E+0	1.2304750E+4 1.0167316E+0

1.2304940E+4 9.9473707E-1	1.2304940E+4 1.0391000E+0	1.2304940E+4 1.0170810E+0
1.2305140E+4 9.9860584E-1	1.2305140E+4 1.0393000E+0	1.2305140E+4 1.0203746E+0
1.2305350E+4 1.0046106E+0	1.2305350E+4 1.0402000E+0	1.2305350E+4 1.0256210E+0
1.2305550E+4 1.0002610E+0	1.2305550E+4 1.0433000E+0	1.2305550E+4 1.0253978E+0
1.2305750E+4 1.0063696E+0	1.2305750E+4 1.0431000E+0	1.2305750E+4 1.0261306E+0
1.2305950E+4 1.0049758E+0	1.2305950E+4 1.0415000E+0	1.2305950E+4 1.0301776E+0
1.2306130E+4 1.0052801E+0	1.2306130E+4 1.0439000E+0	1.2306130E+4 1.0312722E+0
1.2306320E+4 1.0103995E+0	1.2306320E+4 1.0437000E+0	1.2306320E+4 1.0323859E+0
1.2306500E+4 1.0107785E+0	1.2306500E+4 1.0423000E+0	1.2306500E+4 1.0328153E+0
1.2306700E+4 1.0143986E+0	1.2306700E+4 1.0426000E+0	1.2306700E+4 1.0341857E+0
1.2306900E+4 1.0136340E+0	1.2306900E+4 1.0469000E+0	1.2306900E+4 1.0378036E+0
1.2307100E+4 1.0160297E+0	1.2307100E+4 1.0476000E+0	1.2307100E+4 1.0397593E+0
1.2307290E+4 1.0195033E+0	1.2307290E+4 1.0492000E+0	1.2307290E+4 1.0424433E+0
1.2307490E+4 1.0161287E+0	1.2307490E+4 1.0465000E+0	1.2307490E+4 1.0448397E+0
1.2307660E+4 1.0135896E+0	1.2307660E+4 1.0476000E+0	1.2307660E+4 1.0453288E+0
1.2307840E+4 1.0152698E+0	1.2307840E+4 1.0475000E+0	1.2307840E+4 1.0473610E+0
1.2308020E+4 1.0176652E+0	1.2308020E+4 1.0451000E+0	1.2308020E+4 1.0496428E+0
1.2308230E+4 1.0191618E+0	1.2308230E+4 1.0491000E+0	1.2308230E+4 1.0501313E+0
1.2308440E+4 1.0197140E+0	1.2308440E+4 1.0490000E+0	1.2308440E+4 1.0490397E+0
1.2308650E+4 1.0210286E+0	1.2308650E+4 1.0504000E+0	1.2308650E+4 1.0503881E+0
1.2308860E+4 1.0235720E+0	1.2308860E+4 1.0498000E+0	1.2308860E+4 1.0512538E+0
1.2309060E+4 1.0256727E+0	1.2309060E+4 1.0505000E+0	1.2309060E+4 1.0528205E+0
1.2309260E+4 1.0287110E+0	1.2309260E+4 1.0503000E+0	1.2309260E+4 1.0559293E+0
1.2309450E+4 1.0293281E+0	1.2309450E+4 1.0499000E+0	1.2309450E+4 1.0571629E+0
1.2309650E+4 1.0286135E+0	1.2309650E+4 1.0515000E+0	1.2309650E+4 1.0578461E+0
1.2309860E+4 1.0302088E+0	1.2309860E+4 1.0528000E+0	1.2309860E+4 1.0615079E+0
1.2310070E+4 1.0317318E+0	1.2310070E+4 1.0499000E+0	1.2310070E+4 1.0619837E+0
1.2310280E+4 1.0344171E+0	1.2310280E+4 1.0557000E+0	1.2310280E+4 1.0595765E+0
1.2310490E+4 1.0314652E+0	1.2310490E+4 1.0547000E+0	1.2310490E+4 1.0597033E+0
1.2310700E+4 1.0304488E+0	1.2310700E+4 1.0553000E+0	1.2310700E+4 1.0639362E+0
1.2310900E+4 1.0320320E+0	1.2310900E+4 1.0544000E+0	1.2310900E+4 1.0633870E+0
1.2311090E+4 1.0346563E+0	1.2311090E+4 1.0531000E+0	1.2311090E+4 1.0590362E+0
1.2311280E+4 1.0319219E+0	1.2311280E+4 1.0546000E+0	1.2311280E+4 1.0577838E+0
1.2311470E+4 1.0314647E+0	1.2311470E+4 1.0538000E+0	1.2311470E+4 1.0597503E+0
1.2311680E+4 1.0367198E+0	1.2311680E+4 1.0530000E+0	1.2311680E+4 1.0592975E+0
1.2311890E+4 1.0370532E+0	1.2311890E+4 1.0542000E+0	1.2311890E+4 1.0618348E+0
1.2312100E+4 1.0336460E+0	1.2312100E+4 1.0571000E+0	1.2312100E+4 1.0622280E+0
1.2312310E+4 1.0345441E+0	1.2312310E+4 1.0569000E+0	1.2312310E+4 1.0625907E+0
1.2312500E+4 1.0374552E+0	1.2312500E+4 1.0577000E+0	1.2312500E+4 1.0637913E+0
1.2312700E+4 1.0345384E+0	1.2312700E+4 1.0575000E+0	1.2312700E+4 1.0606686E+0
1.2312890E+4 1.0360044E+0	1.2312890E+4 1.0599000E+0	1.2312890E+4 1.0605128E+0
1.2313080E+4 1.0376798E+0	1.2313080E+4 1.0619000E+0	1.2313080E+4 1.0601514E+0
1.2313290E+4 1.0363198E+0	1.2313290E+4 1.0595000E+0	1.2313290E+4 1.0583923E+0
1.2313510E+4 1.0352306E+0	1.2313510E+4 1.0620000E+0	1.2313510E+4 1.0587736E+0
1.2313720E+4 1.0392402E+0	1.2313720E+4 1.0600000E+0	1.2313720E+4 1.0576245E+0
1.2313930E+4 1.0377746E+0	1.2313930E+4 1.0592000E+0	1.2313930E+4 1.0544853E+0
1.2314140E+4 1.0304194E+0	1.2314140E+4 1.0596000E+0	1.2314140E+4 1.0510541E+0
1.2314340E+4 1.0355101E+0	1.2314340E+4 1.0628000E+0	1.2314340E+4 1.0559296E+0
1.2314530E+4 1.0356168E+0	1.2314530E+4 1.0640000E+0	1.2314530E+4 1.0569551E+0
1.2314720E+4 1.0360376E+0	1.2314720E+4 1.0621000E+0	1.2314720E+4 1.0551460E+0
1.2314910E+4 1.0340659E+0	1.2314910E+4 1.0637000E+0	1.2314910E+4 1.0533215E+0
1.2315120E+4 1.0319135E+0	1.2315120E+4 1.0627000E+0	1.2315120E+4 1.0516279E+0



1.2315330E+4	1.0364355E+0	1.2315330E+4	1.0637000E+0	1.2315330E+4	1.0479358E+0
1.2315530E+4	1.0353062E+0	1.2315530E+4	1.0644000E+0	1.2315530E+4	1.0462800E+0
1.2315720E+4	1.0362457E+0	1.2315720E+4	1.0662000E+0	1.2315720E+4	1.0486400E+0
1.2315910E+4	1.0258385E+0	1.2315910E+4	1.0661000E+0	1.2315910E+4	1.0497430E+0
1.2316100E+4	1.0309178E+0	1.2316100E+4	1.0678000E+0	1.2316100E+4	1.0484586E+0
1.2316270E+4	1.0367166E+0	1.2316270E+4	1.0655000E+0	1.2316270E+4	1.0480580E+0
1.2316450E+4	1.0316399E+0	1.2316450E+4	1.0669000E+0	1.2316450E+4	1.0453868E+0
1.2316640E+4	1.0267591E+0	1.2316640E+4	1.0675000E+0	1.2316640E+4	1.0417896E+0
1.2316840E+4	1.0287040E+0	1.2316840E+4	1.0663000E+0	1.2316840E+4	1.0433000E+0
1.2317040E+4	1.0296470E+0	1.2317040E+4	1.0657000E+0	1.2317040E+4	1.0391000E+0
1.2317240E+4	1.0327427E+0	1.2317240E+4	1.0668000E+0	1.2317240E+4	1.0402000E+0
1.2317430E+4	1.0283393E+0	1.2317430E+4	1.0666000E+0	1.2317430E+4	1.0390000E+0
1.2317620E+4	1.0269645E+0	1.2317620E+4	1.0680000E+0	1.2317620E+4	1.0385991E+0
1.2317800E+4	1.0305548E+0	1.2317800E+4	1.0721000E+0	1.2317800E+4	1.0373484E+0
1.2317990E+4	1.0271484E+0	1.2317990E+4	1.0703000E+0	1.2317990E+4	1.0316940E+0
1.2318180E+4	1.0258098E+0	1.2318180E+4	1.0707000E+0	1.2318180E+4	1.0353000E+0
1.2318400E+4	1.0300160E+0	1.2318400E+4	1.0704000E+0	1.2318400E+4	1.0362594E+0
1.2318620E+4	1.0277142E+0	1.2318620E+4	1.0702000E+0	1.2318620E+4	1.0301361E+0
1.2318820E+4	1.0294390E+0	1.2318820E+4	1.0722000E+0	1.2318820E+4	1.0280109E+0
1.2319030E+4	1.0248214E+0	1.2319030E+4	1.0699000E+0	1.2319030E+4	1.0263780E+0
1.2319220E+4	1.0251893E+0	1.2319220E+4	1.0713000E+0	1.2319220E+4	1.0222032E+0
1.2319420E+4	1.0192453E+0	1.2319420E+4	1.0727000E+0	1.2319420E+4	1.0205284E+0
1.2319600E+4	1.0196177E+0	1.2319600E+4	1.0724000E+0	1.2319600E+4	1.0210254E+0
1.2319780E+4	1.0219873E+0	1.2319780E+4	1.0718000E+0	1.2319780E+4	1.0202436E+0
1.2319990E+4	1.0261874E+0	1.2319990E+4	1.0721000E+0	1.2319990E+4	1.0186878E+0
1.2320210E+4	1.0234041E+0	1.2320210E+4	1.0757000E+0	1.2320210E+4	1.0192343E+0
1.2320420E+4	1.0160674E+0	1.2320420E+4	1.0749000E+0	1.2320420E+4	1.0187552E+0
1.2320620E+4	1.0226718E+0	1.2320620E+4	1.0725000E+0	1.2320620E+4	1.0157203E+0
1.2320810E+4	1.0210727E+0	1.2320810E+4	1.0742000E+0	1.2320810E+4	1.0145414E+0
1.2321000E+4	1.0243164E+0	1.2321000E+4	1.0713000E+0	1.2321000E+4	1.0115930E+0
1.2321180E+4	1.0211586E+0	1.2321180E+4	1.0766000E+0	1.2321180E+4	1.0120521E+0
1.2321370E+4	1.0141302E+0	1.2321370E+4	1.0746000E+0	1.2321370E+4	1.0162610E+0
1.2321580E+4	1.0201331E+0	1.2321580E+4	1.0685000E+0	1.2321580E+4	1.0140294E+0
1.2321800E+4	1.0237796E+0	1.2321800E+4	1.0710000E+0	1.2321800E+4	1.0097506E+0
1.2322010E+4	1.0213206E+0	1.2322010E+4	1.0740000E+0	1.2322010E+4	1.0069729E+0
1.2322220E+4	1.0214817E+0	1.2322220E+4	1.0745000E+0	1.2322220E+4	1.0059082E+0
1.2322430E+4	1.0162826E+0	1.2322430E+4	1.0732000E+0	1.2322430E+4	1.0052401E+0
1.2322640E+4	1.0141501E+0	1.2322640E+4	1.0724000E+0	1.2322640E+4	1.0073353E+0
1.2322850E+4	1.0167947E+0	1.2322850E+4	1.0684000E+0	1.2322850E+4	1.0080802E+0
1.2323050E+4	1.0155254E+0	1.2323050E+4	1.0693000E+0	1.2323050E+4	1.0056330E+0
1.2323260E+4	1.0150550E+0	1.2323260E+4	1.0716000E+0	1.2323260E+4	1.0034227E+0
1.2323490E+4	1.0171800E+0	1.2323490E+4	1.0734000E+0	1.2323490E+4	1.0010604E+0
1.2323720E+4	1.0172064E+0	1.2323720E+4	1.0733000E+0	1.2323720E+4	9.9722777E-1
1.2323930E+4	1.0167103E+0	1.2323930E+4	1.0668000E+0	1.2323930E+4	9.9684366E-1
1.2324150E+4	1.0197201E+0	1.2324150E+4	1.0711000E+0	1.2324150E+4	9.9528592E-1
1.2324360E+4	1.0169760E+0	1.2324360E+4	1.0701000E+0	1.2324360E+4	9.9344316E-1
1.2324550E+4	1.0128114E+0	1.2324550E+4	1.0728000E+0	1.2324550E+4	9.9153241E-1
1.2324750E+4	1.0128337E+0	1.2324750E+4	1.0717000E+0	1.2324750E+4	9.9317915E-1
1.2324940E+4	1.0133107E+0	1.2324940E+4	1.0701000E+0	1.2324940E+4	9.9336503E-1
1.2325160E+4	1.0139942E+0	1.2325160E+4	1.0712000E+0	1.2325160E+4	9.9049934E-1
1.2325370E+4	1.0142622E+0	1.2325370E+4	1.0654000E+0	1.2325370E+4	9.9059575E-1
1.2325590E+4	1.0115996E+0	1.2325590E+4	1.0689000E+0	1.2325590E+4	9.8689000E-1

1.2325800E+4	1.0128328E+0	1.2325800E+4	1.0659000E+0	1.2325800E+4	9.8609654E-1
1.2326010E+4	1.0154684E+0	1.2326010E+4	1.0666000E+0	1.2326010E+4	9.8726158E-1
1.2326210E+4	1.0130257E+0	1.2326210E+4	1.0644000E+0	1.2326210E+4	9.8938000E-1
1.2326410E+4	1.0133379E+0	1.2326410E+4	1.0639000E+0	1.2326410E+4	9.8484000E-1
1.2326610E+4	1.0099446E+0	1.2326610E+4	1.0647000E+0	1.2326610E+4	9.8532000E-1
1.2326820E+4	1.0087707E+0	1.2326820E+4	1.0653000E+0	1.2326820E+4	9.8331000E-1
1.2327040E+4	1.0127391E+0	1.2327040E+4	1.0645000E+0	1.2327040E+4	9.8531627E-1
1.2327260E+4	1.0128011E+0	1.2327260E+4	1.0656000E+0	1.2327260E+4	9.8490000E-1
1.2327480E+4	1.0138306E+0	1.2327480E+4	1.0689000E+0	1.2327480E+4	9.8351000E-1
1.2327700E+4	1.0124620E+0	1.2327700E+4	1.0641000E+0	1.2327700E+4	9.8078692E-1
1.2327890E+4	1.0134712E+0	1.2327890E+4	1.0613000E+0	1.2327890E+4	9.7894000E-1
1.2328080E+4	1.0128140E+0	1.2328080E+4	1.0612000E+0	1.2328080E+4	9.7748879E-1
1.2328270E+4	1.0078879E+0	1.2328270E+4	1.0601000E+0	1.2328270E+4	9.7509950E-1
1.2328460E+4	1.0061435E+0	1.2328460E+4	1.0615000E+0	1.2328460E+4	9.7569329E-1
1.2328670E+4	1.0107234E+0	1.2328670E+4	1.0610000E+0	1.2328670E+4	9.7748433E-1
1.2328870E+4	1.0121472E+0	1.2328870E+4	1.0607000E+0	1.2328870E+4	9.7407536E-1
1.2329080E+4	1.0085582E+0	1.2329080E+4	1.0582000E+0	1.2329080E+4	9.7234061E-1
1.2329280E+4	1.0018089E+0	1.2329280E+4	1.0574000E+0	1.2329280E+4	9.7219898E-1
1.2329470E+4	1.0064000E+0	1.2329470E+4	1.0559000E+0	1.2329470E+4	9.6975120E-1
1.2329650E+4	1.0087796E+0	1.2329650E+4	1.0526000E+0	1.2329650E+4	9.6747990E-1
1.2329830E+4	1.0082948E+0	1.2329830E+4	1.0563000E+0	1.2329830E+4	9.6706904E-1
1.2330010E+4	1.0064751E+0	1.2330010E+4	1.0521000E+0	1.2330010E+4	9.6956497E-1
1.2330210E+4	1.0052444E+0	1.2330210E+4	1.0572000E+0	1.2330210E+4	9.7125253E-1
1.2330410E+4	1.0052638E+0	1.2330410E+4	1.0534000E+0	1.2330410E+4	9.6967735E-1
1.2330610E+4	1.0044065E+0	1.2330610E+4	1.0545000E+0	1.2330610E+4	9.7018997E-1
1.2330820E+4	9.9570524E-1	1.2330820E+4	1.0517000E+0	1.2330820E+4	9.6560833E-1
1.2331010E+4	9.9752727E-1	1.2331010E+4	1.0505000E+0	1.2331010E+4	9.6216056E-1
1.2331200E+4	1.0073349E+0	1.2331200E+4	1.0508000E+0	1.2331200E+4	9.6135637E-1
1.2331380E+4	1.0014592E+0	1.2331380E+4	1.0458000E+0	1.2331380E+4	9.6034390E-1
1.2331560E+4	9.9590550E-1	1.2331560E+4	1.0500000E+0	1.2331560E+4	9.5712443E-1
1.2331780E+4	9.9919449E-1	1.2331780E+4	1.0426000E+0	1.2331780E+4	9.5885690E-1
1.2331990E+4	1.0002085E+0	1.2331990E+4	1.0453000E+0	1.2331990E+4	9.5863953E-1
1.2332200E+4	1.0022482E+0	1.2332200E+4	1.0442000E+0	1.2332200E+4	9.5590186E-1
1.2332400E+4	9.9699657E-1	1.2332400E+4	1.0410000E+0	1.2332400E+4	9.5557247E-1
1.2332600E+4	9.9372103E-1	1.2332600E+4	1.0447000E+0	1.2332600E+4	9.5747789E-1
1.2332800E+4	9.9858972E-1	1.2332800E+4	1.0404000E+0	1.2332800E+4	9.5323186E-1
1.2332990E+4	9.9831096E-1	1.2332990E+4	1.0424000E+0	1.2332990E+4	9.4849428E-1
1.2333170E+4	9.9417951E-1	1.2333170E+4	1.0409000E+0	1.2333170E+4	9.5003728E-1
1.2333360E+4	9.9133542E-1	1.2333360E+4	1.0370000E+0	1.2333360E+4	9.4753550E-1
1.2333560E+4	9.8836236E-1	1.2333560E+4	1.0382000E+0	1.2333560E+4	9.4976401E-1
1.2333760E+4	9.8998153E-1	1.2333760E+4	1.0372000E+0	1.2333760E+4	9.5092024E-1
1.2333970E+4	9.8856651E-1	1.2333970E+4	1.0375000E+0	1.2333970E+4	9.4734175E-1
1.2334160E+4	9.8460604E-1	1.2334160E+4	1.0367000E+0	1.2334160E+4	9.4815120E-1
1.2334350E+4	9.8687633E-1	1.2334350E+4	1.0342000E+0	1.2334350E+4	9.4906485E-1
1.2334530E+4	9.8766416E-1	1.2334530E+4	1.0304000E+0	1.2334530E+4	9.4693988E-1
1.2334710E+4	9.8817555E-1	1.2334710E+4	1.0302000E+0	1.2334710E+4	9.4745151E-1
1.2334900E+4	9.8647784E-1	1.2334900E+4	1.0261000E+0	1.2334900E+4	9.4726628E-1
1.2335110E+4	9.7904864E-1	1.2335110E+4	1.0322000E+0	1.2335110E+4	9.4499406E-1
1.2335320E+4	9.7851790E-1	1.2335320E+4	1.0306000E+0	1.2335320E+4	9.4365705E-1
1.2335540E+4	9.8290314E-1	1.2335540E+4	1.0266000E+0	1.2335540E+4	9.4406350E-1
1.2335750E+4	9.8296754E-1	1.2335750E+4	1.0266000E+0	1.2335750E+4	9.4084689E-1
1.2335960E+4	9.8222505E-1	1.2335960E+4	1.0263000E+0	1.2335960E+4	9.4031000E-1

1.2336160E+4 9.8262146E-1	1.2336160E+4 1.0267000E+0	1.2336160E+4 9.4092316E-1
1.2336360E+4 9.8300100E-1	1.2336360E+4 1.0279000E+0	1.2336360E+4 9.3892696E-1
1.2336560E+4 9.8592803E-1	1.2336560E+4 1.0243000E+0	1.2336560E+4 9.3967476E-1
1.2336760E+4 9.8405362E-1	1.2336760E+4 1.0236000E+0	1.2336760E+4 9.4011352E-1
1.2336980E+4 9.7823389E-1	1.2336980E+4 1.0232000E+0	1.2336980E+4 9.3550834E-1
1.2337200E+4 9.8008646E-1	1.2337200E+4 1.0205000E+0	1.2337200E+4 9.3893177E-1
1.2337410E+4 9.7785848E-1	1.2337410E+4 1.0211000E+0	1.2337410E+4 9.3733495E-1
1.2337620E+4 9.7806793E-1	1.2337620E+4 1.0194000E+0	1.2337620E+4 9.3965788E-1
1.2337810E+4 9.7692340E-1	1.2337810E+4 1.0143000E+0	1.2337810E+4 9.3529721E-1
1.2338010E+4 9.7397787E-1	1.2338010E+4 1.0154000E+0	1.2338010E+4 9.3994579E-1
1.2338190E+4 9.7303116E-1	1.2338190E+4 1.0138000E+0	1.2338190E+4 9.3756650E-1
1.2338390E+4 9.7610944E-1	1.2338390E+4 1.0151000E+0	1.2338390E+4 9.3702122E-1
1.2338590E+4 9.7312640E-1	1.2338590E+4 1.0167000E+0	1.2338590E+4 9.3800623E-1
1.2338800E+4 9.7291921E-1	1.2338800E+4 1.0147000E+0	1.2338800E+4 9.3755492E-1
1.2339010E+4 9.7307316E-1	1.2339010E+4 1.0114000E+0	1.2339010E+4 9.3394696E-1
1.2339210E+4 9.7153849E-1	1.2339210E+4 1.0141000E+0	1.2339210E+4 9.3309048E-1
1.2339420E+4 9.7395720E-1	1.2339420E+4 1.0117000E+0	1.2339420E+4 9.3106181E-1
1.2339620E+4 9.7184939E-1	1.2339620E+4 1.0129000E+0	1.2339620E+4 9.3572573E-1
1.2339810E+4 9.6894414E-1	1.2339810E+4 1.0104000E+0	1.2339810E+4 9.3922547E-1
1.2340000E+4 9.7306298E-1	1.2340000E+4 1.0108000E+0	1.2340000E+4 9.3557098E-1
1.2340210E+4 9.7697689E-1	1.2340210E+4 1.0085000E+0	1.2340210E+4 9.3844110E-1
1.2340410E+4 9.7637099E-1	1.2340410E+4 1.0069000E+0	1.2340410E+4 9.3657223E-1
1.2340630E+4 9.7369690E-1	1.2340630E+4 1.0061000E+0	1.2340630E+4 9.3714355E-1
1.2340840E+4 9.6884136E-1	1.2340840E+4 1.0057000E+0	1.2340840E+4 9.3975568E-1
1.2341040E+4 9.6766300E-1	1.2341040E+4 1.0051000E+0	1.2341040E+4 9.3348701E-1
1.2341230E+4 9.6848915E-1	1.2341230E+4 1.0034000E+0	1.2341230E+4 9.3349617E-1
1.2341420E+4 9.7001455E-1	1.2341420E+4 1.0023000E+0	1.2341420E+4 9.3629316E-1
1.2341600E+4 9.6925071E-1	1.2341600E+4 9.9830000E-1	1.2341600E+4 9.3456015E-1
1.2341790E+4 9.6577750E-1	1.2341790E+4 1.0016000E+0	1.2341790E+4 9.3369138E-1
1.2341980E+4 9.6721969E-1	1.2341980E+4 1.0023000E+0	1.2341980E+4 9.3783008E-1
1.2342190E+4 9.6891897E-1	1.2342190E+4 1.0014000E+0	1.2342190E+4 9.4114975E-1
1.2342390E+4 9.6739433E-1	1.2342390E+4 1.0046000E+0	1.2342390E+4 9.3648474E-1
1.2342580E+4 9.6591232E-1	1.2342580E+4 9.9994000E-1	1.2342580E+4 9.3578145E-1
1.2342770E+4 9.6793307E-1	1.2342770E+4 1.0006000E+0	1.2342770E+4 9.3675000E-1
1.2342950E+4 9.7048579E-1	1.2342950E+4 9.9703000E-1	1.2342950E+4 9.3716585E-1
1.2343130E+4 9.7361430E-1	1.2343130E+4 1.0010000E+0	1.2343130E+4 9.3671787E-1
1.2343310E+4 9.7508108E-1	1.2343310E+4 9.9693000E-1	1.2343310E+4 9.4202586E-1
1.2343500E+4 9.7191355E-1	1.2343500E+4 9.9880000E-1	1.2343500E+4 9.4180317E-1
1.2343690E+4 9.7053433E-1	1.2343690E+4 9.9804000E-1	1.2343690E+4 9.4130137E-1
1.2343900E+4 9.6531959E-1	1.2343900E+4 1.0003000E+0	1.2343900E+4 9.4122427E-1
1.2344110E+4 9.6713527E-1	1.2344110E+4 9.9791000E-1	1.2344110E+4 9.4116386E-1
1.2344310E+4 9.6541697E-1	1.2344310E+4 1.0006000E+0	1.2344310E+4 9.4116542E-1
1.2344500E+4 9.6805378E-1	1.2344500E+4 9.9797000E-1	1.2344500E+4 9.4287414E-1
1.2344680E+4 9.6710047E-1	1.2344680E+4 9.9740000E-1	1.2344680E+4 9.4466997E-1
1.2344860E+4 9.7091989E-1	1.2344860E+4 9.9687000E-1	1.2344860E+4 9.4253212E-1
1.2345060E+4 9.7155279E-1	1.2345060E+4 9.9977000E-1	1.2345060E+4 9.4508776E-1
1.2345280E+4 9.7251787E-1	1.2345280E+4 9.9847000E-1	1.2345280E+4 9.4493273E-1
1.2345500E+4 9.6796112E-1	1.2345500E+4 9.9766000E-1	1.2345500E+4 9.4487357E-1
1.2345710E+4 9.6993110E-1	1.2345710E+4 9.9765000E-1	1.2345710E+4 9.5020121E-1
1.2345910E+4 9.7389000E-1	1.2345910E+4 9.9451000E-1	1.2345910E+4 9.5238556E-1
1.2346110E+4 9.7065001E-1	1.2346110E+4 9.9306000E-1	1.2346110E+4 9.5189498E-1
1.2346290E+4 9.7581215E-1	1.2346290E+4 9.9574000E-1	1.2346290E+4 9.5290719E-1

1.2346480E+4 9.7063867E-1	1.2346480E+4 9.9269000E-1	1.2346480E+4 9.5021231E-1
1.2346670E+4 9.7116442E-1	1.2346670E+4 9.9532000E-1	1.2346670E+4 9.5091612E-1
1.2346870E+4 9.7051394E-1	1.2346870E+4 9.9297000E-1	1.2346870E+4 9.5734583E-1
1.2347070E+4 9.7196103E-1	1.2347070E+4 9.9396000E-1	1.2347070E+4 9.5645109E-1
1.2347270E+4 9.7350824E-1	1.2347270E+4 9.9353000E-1	1.2347270E+4 9.5416052E-1
1.2347460E+4 9.7807567E-1	1.2347460E+4 9.9594000E-1	1.2347460E+4 9.5415447E-1
1.2347650E+4 9.7803327E-1	1.2347650E+4 9.9620000E-1	1.2347650E+4 9.5675466E-1
1.2347840E+4 9.8323115E-1	1.2347840E+4 9.9411000E-1	1.2347840E+4 9.5555223E-1
1.2348020E+4 9.8006668E-1	1.2348020E+4 9.9968000E-1	1.2348020E+4 9.6499000E-1
1.2348210E+4 9.7530530E-1	1.2348210E+4 9.9547000E-1	1.2348210E+4 9.6144017E-1
1.2348420E+4 9.7968684E-1	1.2348420E+4 9.9599000E-1	1.2348420E+4 9.5924313E-1
1.2348630E+4 9.8552138E-1	1.2348630E+4 9.9277000E-1	1.2348630E+4 9.6299768E-1
1.2348860E+4 9.8228814E-1	1.2348860E+4 9.9262000E-1	1.2348860E+4 9.6264118E-1
1.2349070E+4 9.8254008E-1	1.2349070E+4 9.9671000E-1	1.2349070E+4 9.6368343E-1
1.2349280E+4 9.8047151E-1	1.2349280E+4 9.9428000E-1	1.2349280E+4 9.6809003E-1
1.2349490E+4 9.8340840E-1	1.2349490E+4 9.9606000E-1	1.2349490E+4 9.6741195E-1
1.2349680E+4 9.8254469E-1	1.2349680E+4 9.9725000E-1	1.2349680E+4 9.6714711E-1
1.2349890E+4 9.8280529E-1	1.2349890E+4 9.9430000E-1	1.2349890E+4 9.6856203E-1
1.2350090E+4 9.8510954E-1	1.2350090E+4 9.9379000E-1	1.2350090E+4 9.7053083E-1
1.2350300E+4 9.8684687E-1	1.2350300E+4 9.9815000E-1	1.2350300E+4 9.7187891E-1
1.2350530E+4 9.8371963E-1	1.2350530E+4 9.9822000E-1	1.2350530E+4 9.7487000E-1
1.2350740E+4 9.8597546E-1	1.2350740E+4 9.9636000E-1	1.2350740E+4 9.7770725E-1
1.2350950E+4 9.8700799E-1	1.2350950E+4 9.9441000E-1	1.2350950E+4 9.7228000E-1
1.2351160E+4 9.8428214E-1	1.2351160E+4 9.9277000E-1	1.2351160E+4 9.8030000E-1
1.2351360E+4 9.8605860E-1	1.2351360E+4 9.9586000E-1	1.2351360E+4 9.7586000E-1
1.2351550E+4 9.8935245E-1	1.2351550E+4 9.9649000E-1	1.2351550E+4 9.8111000E-1
1.2351740E+4 9.8434586E-1	1.2351740E+4 9.9490000E-1	1.2351740E+4 9.7861582E-1
1.2351960E+4 9.8710958E-1	1.2351960E+4 9.9899000E-1	1.2351960E+4 9.8006822E-1
1.2352180E+4 9.8871933E-1	1.2352180E+4 9.9995000E-1	1.2352180E+4 9.7894229E-1
1.2352400E+4 9.9138496E-1	1.2352400E+4 9.9861000E-1	1.2352400E+4 9.8148433E-1
1.2352620E+4 9.8292110E-1	1.2352620E+4 9.9935000E-1	1.2352620E+4 9.8640931E-1
1.2352820E+4 9.9620000E-1	1.2352820E+4 9.9606000E-1	1.2352820E+4 9.7915990E-1
1.2353030E+4 9.8931352E-1	1.2353030E+4 1.0002000E+0	1.2353030E+4 9.8458925E-1
1.2353230E+4 9.9294347E-1	1.2353230E+4 9.9987000E-1	1.2353230E+4 9.8319000E-1
1.2353420E+4 9.9982944E-1	1.2353420E+4 9.9792000E-1	1.2353420E+4 9.8920478E-1
1.2353620E+4 9.9428754E-1	1.2353620E+4 9.9308000E-1	1.2353620E+4 9.8737361E-1
1.2353840E+4 9.9138978E-1	1.2353840E+4 9.9746000E-1	1.2353840E+4 9.8729442E-1
1.2354060E+4 1.0005498E+0	1.2354060E+4 1.0041000E+0	1.2354060E+4 9.9043803E-1
1.2354290E+4 1.0002770E+0	1.2354290E+4 1.0023000E+0	1.2354290E+4 9.8736504E-1
1.2354500E+4 9.9915768E-1	1.2354500E+4 1.0001000E+0	1.2354500E+4 9.9447582E-1
1.2354690E+4 9.9310406E-1	1.2354690E+4 1.0033000E+0	1.2354690E+4 9.9242647E-1
1.2354890E+4 9.9431248E-1	1.2354890E+4 1.0019000E+0	1.2354890E+4 9.8785946E-1
1.2355070E+4 9.9391373E-1	1.2355070E+4 1.0001000E+0	1.2355070E+4 9.9035980E-1
1.2355270E+4 9.9841193E-1	1.2355270E+4 9.9911000E-1	1.2355270E+4 9.9711205E-1
1.2355470E+4 1.0026877E+0	1.2355470E+4 9.9935000E-1	1.2355470E+4 9.9803689E-1
1.2355680E+4 1.0030919E+0	1.2355680E+4 1.0027000E+0	1.2355680E+4 9.9343688E-1
1.2355890E+4 1.0019789E+0	1.2355890E+4 1.0010000E+0	1.2355890E+4 9.9688746E-1
1.2356080E+4 1.0021151E+0	1.2356080E+4 1.0041000E+0	1.2356080E+4 9.9568639E-1
1.2356280E+4 9.9663589E-1	1.2356280E+4 1.0008000E+0	1.2356280E+4 9.9550696E-1
1.2356470E+4 9.9653085E-1	1.2356470E+4 9.9979000E-1	1.2356470E+4 9.9883983E-1
1.2356660E+4 1.0005198E+0	1.2356660E+4 1.0049000E+0	1.2356660E+4 9.9642782E-1
1.2356850E+4 1.0011126E+0	1.2356850E+4 1.0030000E+0	1.2356850E+4 9.9704429E-1

1.2357040E+4	1.0013385E+0	1.2357040E+4	1.0036000E+0	1.2357040E+4	1.0004405E+0
1.2357250E+4	1.0052023E+0	1.2357250E+4	1.0022000E+0	1.2357250E+4	9.9639253E-1
1.2357470E+4	1.0067368E+0	1.2357470E+4	1.0088000E+0	1.2357470E+4	9.9847499E-1
1.2357690E+4	1.0059824E+0	1.2357690E+4	9.9991000E-1	1.2357690E+4	1.0025778E+0
1.2357900E+4	1.0052340E+0	1.2357900E+4	1.0056000E+0	1.2357900E+4	1.0031839E+0
1.2358100E+4	1.0009322E+0	1.2358100E+4	1.0013000E+0	1.2358100E+4	9.9602643E-1
1.2358280E+4	1.0019618E+0	1.2358280E+4	1.0024000E+0	1.2358280E+4	9.9904170E-1
1.2358390E+4	1.0053000E+0	1.2358390E+4	1.0049000E+0	1.2358390E+4	1.0055058E+0
1.2358420E+4	1.0062868E+0	1.2358420E+4	1.0036000E+0	1.2358420E+4	1.0069877E+0
1.2358440E+4	1.0069265E+0	1.2358440E+4	1.0020000E+0	1.2358440E+4	1.0078017E+0

## 5. Optimized Cartesian coordinates

### CysSerGlyCysLys

S	-0.34157337381242	-0.76003187338060	3.57994755253456
S	-3.01352745840693	0.24460605856372	6.72659753983417
O	-1.63354595384508	4.68795957178038	2.68001058926802
O	-1.45558383212022	0.45689419977587	-0.35690064141965
O	-3.76669102208535	-0.50481595170180	3.76003494799486
O	1.46507533348402	4.63626859184317	4.07883085103340
O	-3.18710464626939	2.41908729081182	3.86096488282802
O	-3.00367615552067	-5.19306068573532	3.73495800246666
N	-3.61381982896932	-2.66869666532016	3.08744084649658
N	-2.42360943339087	0.45814657749549	1.69832748577436
N	-1.75787565252392	3.39427235270269	5.33398309940224
N	-5.19582040806730	3.53712065789638	5.70797689216658
N	-0.75597360183960	2.65175394515542	2.16952522998632
N	-8.63658302182973	-0.11191462704052	3.86179233667660
N	-3.64164967044684	-4.88520831373181	5.89127914700474
C	-0.60609866521299	3.42450216728867	4.45460005366135
C	-2.43488990649009	-0.98164956636849	1.81584767111378
C	-1.78314703381459	1.05291134064029	0.67244580342031
C	-1.01809453351152	-1.51848854891819	2.06198243867951
C	-3.34882035557608	-1.35458457310343	2.97691048244739
C	-4.26684225250485	-3.21972150618944	4.25393165654316
C	-1.06371993749884	3.65370178150595	3.01635278000668
C	0.30223712055578	4.56858121066608	4.88728523077931
C	-2.93648907133654	2.83770666665165	4.99379751738527
C	-3.56299128181023	-4.52095933863969	4.60503585556027
C	-3.99915899175350	2.78405675043982	6.08182754126442
C	-4.39718839447278	1.32787806143745	6.27960324652599
C	-1.43023714310760	2.51530653689614	0.89092023311449
C	-5.75326318459425	-3.50444719593526	3.99523555661549
C	-6.54930744777361	-2.24596988436389	3.66549228721479
C	-6.74761496831400	-1.33262231826429	4.86914018283315
C	-7.32065458213151	0.02560641268356	4.49854389998043
H	-2.67419934343945	0.99411405332260	2.53307397841841
H	-2.80794600923194	-1.43193120090833	0.89106658412467
H	-3.20534081595053	-3.33577403719382	2.44311524288358
H	-0.38601082747737	1.80206280054391	2.58371631580289
H	0.55766003040002	4.45043320737536	5.94540233444099
H	-0.05549674466528	2.47752242414037	4.52466608289763
H	-0.38587383962612	-1.25325756218247	1.21527766976984

H	-3.61038155673984	3.19682212070656	7.01742386241379
H	-1.61358887065169	3.64321130744197	6.30410093400468
H	-4.15169835968338	-2.49565683532327	5.06527266455760
H	-1.03671220747382	-2.60421683376974	2.16523073167068
H	-5.48659269229382	3.23124999091616	4.78032674848858
H	-5.18884088268514	1.25897004554709	7.02638492391173
H	-4.75951878541307	0.93046101894870	5.33036797001537
H	-9.01491246124628	0.81448858387905	3.68022177460375
H	-9.27561778550600	-0.53634152008228	4.53081499675193
H	-7.35213058713340	0.65920877763908	5.39478984462986
H	-6.64603355380169	0.50985864493358	3.78459074305613
H	-5.79169083097520	-1.16600366329607	5.37295861857332
H	-7.41012751187101	-1.82198068095249	5.59448103856569
H	-6.04228736585390	-1.69311961043449	2.86722961083392
H	-7.52284619169126	-2.53988176191667	3.26682281673460
H	-5.81184821673487	-4.21997621271657	3.16797034561234
H	-6.17840199500167	-3.99371691585686	4.87856861487783
H	2.04675533720517	3.90506961545800	4.33109258006911
H	-0.23357132617423	5.50943048876997	4.75652496389112
H	-0.80612235799352	2.83555456476572	0.05604281803661
H	-2.33284355199281	3.13260263344514	0.91226199748626
H	-4.09539700507763	-4.30427382251481	6.57835699797370
H	-3.26590547616746	-5.77553699145957	6.18532059647147
H	-4.96202975837387	4.52389275829961	5.61642820343413
H	-2.85638682616546	0.71556588684149	7.97325317881372
H	0.92357072447738	-1.14889039990852	3.37144901699077

### Hg(CysSerGlyCysLys)

Hg	-1.36350307996235	0.04725582175852	5.53429718831469
S	0.11506807319511	-0.34703600804549	3.79309418088947
S	-2.54602997391056	0.59119016257166	7.44399952511969
O	-2.31409951002811	4.42173512275006	2.45559525325353
O	-1.26520565879811	0.01506084814782	-0.07852129542817
O	-3.40453382533704	-0.95739321400266	4.24717678372658
O	0.86068101229851	5.26017117800557	3.47165186539054
O	-3.08463313448987	2.02854182443431	4.14827081644182
O	-3.75716654885241	-5.56107108819941	3.08010513548529
N	-3.67629129506993	-2.86925151560342	3.05446986357719
N	-2.28291476382536	0.18187589495045	1.94623880600931
N	-1.91284927318091	3.62955744686466	5.24277890110222
N	-5.24305397667175	3.22235965824646	5.84356952035004
N	-0.93400813779498	2.64465401488384	2.09663207591342
N	-8.21276719697277	0.47547856882056	3.87661113178812
N	-4.46668032544731	-5.57233276741286	5.23747007959799
C	-0.86368156509011	3.73578765811957	4.24888006469323
C	-2.12706962985180	-1.22516261624206	2.22695253070241
C	-1.68668462785313	0.70451806407682	0.85163205227448
C	-0.70055522514856	-1.57496710101149	2.71552171943569
C	-3.14097354835193	-1.66050366748683	3.26086338450639
C	-4.57462838168151	-3.50236038543276	3.99457819014758
C	-1.46035559511857	3.63041575630959	2.84717825152493
C	-0.18732655003498	5.09334260250728	4.40932745151940

C	-2.93203589254795	2.76475518887220	5.13356463512723
C	-4.20925006256113	-4.97627961545639	4.06712664703935
C	-3.93391218907711	2.72898600209761	6.27319017160942
C	-4.08089076490809	1.28545009811974	6.73706042611451
C	-1.53897053477159	2.21755449045145	0.85127854007629
C	-6.03541964595135	-3.37866650120295	3.53640394673846
C	-6.50558261588495	-1.93427084269757	3.41000639326257
C	-6.65950780103167	-1.22824581033012	4.75066788363228
C	-6.95756271588378	0.25473095568117	4.60463455805730
H	-2.51524986174639	0.79832904043313	2.72635803077882
H	-2.28803873651974	-1.78113698627960	1.29999391855035
H	-3.42954622440561	-3.40082498459950	2.22746004597478
H	-0.32458731467517	1.97906753829742	2.56257683398722
H	0.17330673150100	5.19880556259472	5.43760185673553
H	-0.12049409837208	2.94226622892223	4.40079325565429
H	-0.04426057585701	-1.63058438566508	1.84383959555195
H	-3.58637485313883	3.34791177831463	7.10496788377124
H	-1.82265036936645	4.16307542314975	6.09870027567448
H	-4.43054064627004	-3.02055192987903	4.96359603171111
H	-0.70553419681057	-2.55602885114149	3.19558906093298
H	-5.51415051137272	2.72830276048247	4.99536934358311
H	-4.82535893817405	1.24642201224573	7.53555628044798
H	-4.41379344090048	0.66060525630167	5.90650222070707
H	-8.40872835635519	1.47297697037762	3.84500420503094
H	-8.97430397329474	0.06952440091677	4.41647688613116
H	-6.96119216676674	0.71926593068914	5.59902185323484
H	-6.14611422927439	0.71730149376074	4.03148512263941
H	-5.74004420071348	-1.32754459660909	5.33425409939963
H	-7.46119046708390	-1.70630693788763	5.32766627373404
H	-5.80362381830323	-1.37393545137956	2.78172382064087
H	-7.46204542465500	-1.92412969363933	2.88275410300797
H	-6.12101503766458	-3.89005204982750	2.57159121432999
H	-6.66982107628927	-3.91881807604226	4.24748224427269
H	1.61085122100083	4.72184100365796	3.76184276002720
H	-0.92267930308497	5.87443720797092	4.21123129688883
H	-0.93468959539605	2.49167146489561	-0.01415927229744
H	-2.51685956447246	2.69804323347949	0.76501279129618
H	-4.80647573136032	-5.05213451177902	6.03094982241534
H	-4.32108736373368	-6.56697666008227	5.33708132963334
H	-5.16877991584858	4.20514758377599	5.58722513756086

**[Hg(PC2)]<sup>-2</sup>**

Hg	-2.54973949755173	0.29785811772234	6.58831176265402
S	-0.52912023697255	-0.82656100784523	6.69666697002173
S	-4.39148313292006	1.61852518833407	7.06704003332646
O	1.49224052527581	-0.67988369053712	3.74598250906823
O	-3.32192004203707	-1.11390088744993	4.48256270432593
O	-2.51927956562524	4.53548554436716	1.93094811396859
O	-0.50583051961776	4.79678792385199	0.96924300985446
O	-2.57951056660225	1.78196569435313	4.03752782662809
O	-5.66893261139761	-5.29578482138611	2.61447099415858
O	-3.43950330233348	-5.39596153884081	2.29005173894923

O	-5.21960748613979	5.91136081759845	5.67103110624623
O	-6.52394390318605	8.67824078398019	1.09145035459072
O	-4.29525349374361	9.05366745889031	1.10522747660159
N	-2.97486849950492	-3.08503340302986	3.42367848425913
N	-0.75630157028031	-0.39889240008721	3.67848381195387
N	-1.40568636726468	3.73282182405624	4.27852371595599
N	-4.09356336712577	4.56059240958462	4.22927411854579
N	-3.63095263560256	6.61870667494080	0.54763452714381
C	-1.05145943416468	-1.76436427607851	4.03474680351164
C	0.51154661148246	0.07046117242600	3.71945502230550
C	0.62284807687742	1.57678827397116	3.77833096871858
C	-0.55620334149658	3.71995767895267	3.08758275741601
C	-0.56293184896410	-2.15596635793900	5.45267319638887
C	-2.55331903760909	-1.95516356559224	3.98074281769021
C	-4.36427507185936	-3.48322724194139	3.38294554399520
C	-0.10294944242966	2.32451767425537	2.65541242165255
C	-1.24752403675815	4.41949143111271	1.89248339953445
C	-2.46513397817608	2.92707249577542	4.48300832344195
C	-4.49824933638294	-4.85220371407219	2.69869459001690
C	-3.63487945500249	3.59244351175681	5.21424142508836
C	-4.72308255919804	2.58916560136752	5.55966421574984
C	-4.76288441669084	5.68692156939751	4.54622650131043
C	-4.85654250267124	6.66294541540910	3.38943145866780
C	-5.07851547031405	6.81674731606363	0.85415494815231
C	-5.32523582584447	8.33173908951672	1.02095130305440
C	-5.47500546035681	6.06458602441115	2.11893888762770
H	-1.50561602567082	0.28334523822499	3.79433419629236
H	0.56913521416595	2.46028094547710	1.80567470892558
H	-0.96482070928497	1.76278196603427	2.29897440895835
H	-0.56528989054404	-2.44609252392842	3.33094761849135
H	-2.33263111601969	-3.74381768712804	2.99480289730187
H	0.19992842308937	1.86998747745661	4.74582471381049
H	0.32728503365684	4.31322255611533	3.33801091274772
H	1.68251649085147	1.83506264718803	3.79217254438142
H	0.47847899396929	-2.47540935267711	5.38992697412036
H	-3.30063921890924	4.11350962279626	6.11940325039577
H	-1.49547777926368	4.65123865657686	4.69855637010479
H	-4.95837104638284	-2.74942665956844	2.83263422474901
H	-4.77428570587839	-3.54552235309883	4.39400338946198
H	-1.15634300042453	-2.99876180284825	5.81391825315444
H	-3.60287708004904	4.54087634971120	3.32471126110731
H	-5.63908934216042	3.14008847117782	5.78367353330707
H	-4.90030535758797	1.92839149147119	4.71105190186293
H	-3.83348250984287	7.00367185785306	3.19134506195637
H	-5.42761733988851	7.53090614299076	3.71970414257398
H	-5.19595945703669	5.01574134345323	1.99798736730561
H	-6.56333629697083	6.09681073532739	2.19498222751090
H	-5.65683293865047	6.44430866322643	0.00955930857044
H	-3.48595735416124	6.50554734448207	-0.45542753770425
H	-3.18013519086417	7.50814089141127	0.81775190233255
H	-3.18285699395420	5.79442319097976	1.03392452570643



**[Hg<sub>3</sub>(SMe)<sub>9</sub>]<sup>-3-β</sup>**

Hg	-2.27076471606678	1.46492430844317	-0.40639654853980
Hg	-2.60700025410234	-2.17157725613512	-1.68940272266850
Hg	-2.77548910686926	0.75133156907018	-4.00747099198925
S	0.03046037026807	0.67729553041501	-0.03278811584684
S	-2.33290230288620	2.86246025297513	-2.54100275003822
S	-3.96466820414657	-0.42707535607536	-0.42233472854507
S	-3.07297029469184	3.03058150301236	1.39516237654693
S	-3.99307224686016	-3.55218111049569	-3.20504832613198
S	-1.21647015356539	-3.45313746755834	-0.09927780875239
S	-1.00849356761074	-0.86978241951699	-3.25079529545371
S	-1.96204752387824	1.53802435063076	-6.25714304881772
S	-5.15977550621620	0.26289298736997	-3.86779272491766
C	0.67148670829717	2.22239590944598	0.71061403657675
C	-2.27220788169437	4.56992775766662	0.81981711277806
C	-2.53180442308095	3.27320783956417	-6.21582834741479
C	-5.73619279686431	1.56754236922663	-5.01670924464760
C	-1.07225415244773	-1.95856717546307	-4.71708859729636
C	0.42396719328246	-3.13901532973084	-0.83868064117846
C	-2.88732216232118	-5.00566599706437	-3.30962360385357
C	-0.54523593850291	3.01652587130674	-2.87116007646741
C	-3.62679843881803	-0.98086699939779	1.28752673329987
H	1.68160845268391	2.04846277604065	1.08799072924783
H	0.70992386478038	3.02448417933379	-0.02942192657440
H	0.03667323138615	2.54738355015313	1.53662860190202
H	-2.75264032708214	5.43013872784607	1.28990421480964
H	-1.21218519513932	4.57885747355837	1.07755392554431
H	-2.36399892467631	4.65964804890140	-0.26433929056875
H	-2.03324004127528	3.83793693844594	-7.00613108694404
H	-3.61012019967900	3.33668170458002	-6.36893031223870
H	-2.29771110959904	3.73003452573241	-5.25254245383106
H	-5.24008689701120	1.47817308394814	-5.98437763162879
H	-6.81377021888165	1.46557900729979	-5.16152245213909
H	-5.53055083055063	2.56127353231328	-4.61543247267293
H	-0.31961036609731	-2.74304464658047	-4.61274615200707
H	-2.06035440018064	-2.41556852647535	-4.79901351255891
H	-0.85764439841833	-1.37439324835809	-5.61397746868989
H	0.63459376030093	-2.06947040442052	-0.84103240102314
H	1.18330614542609	-3.65593524851509	-0.24762081309922
H	0.46738070106063	-3.50567648446508	-1.86533268160324
H	-3.43153500689019	-5.84784396165549	-3.74149801450648
H	-2.02575280736756	-4.78637590278241	-3.94373991280831
H	-2.52028821065118	-5.28506496436283	-2.32130463686686
H	-0.16498638969794	3.93717982898423	-2.42410945085395
H	-0.02142767289972	2.16010742789948	-2.44089474209122
H	-0.38113680305265	3.03822232363786	-3.95047704235275
H	-2.57483935728852	-1.24616527853597	1.39206954019965
H	-3.87952249905053	-0.17729302766775	1.98143491554929
H	-4.23948738137343	-1.85549251254460	1.51308083116370

**[Hg<sub>4</sub>(SMe)<sub>11</sub>]<sup>-3-α</sup>**

Hg	-1.93466988232515	0.53967650243005	-0.19815103427565
Hg	-1.53885459171021	1.77617421170769	-3.79131206387340
Hg	-0.40715132113684	-2.18144965496310	-2.77456397512833
Hg	-3.50624510479497	-3.50089137671789	-0.27250156168152
S	0.31988871867107	2.74882261281709	-2.56044383447339
S	0.13654950477432	-0.72667572652281	-0.72418567024094
S	-1.86391304903162	2.54052047025228	1.22539875101162
S	-0.55486580748830	-0.49740844514592	-4.64282568375297
S	-2.75711413054068	2.63052269455416	-5.74402382451248
S	-3.45621406927808	1.16486569849202	-2.12476540105201
S	-2.47402476348554	-3.55792388366665	-2.64810637392728
S	1.61402467231458	-3.59740061169663	-2.88936021856328
S	-2.27227403091114	-5.18489234341913	1.03932526673407
S	-3.38301178199874	-1.28546616597856	0.97833123060039
S	-5.92220889181345	-3.90732926448893	-0.59801240429934
C	1.68061892772504	1.65752321230669	-3.10547924566395
C	0.11144445972144	-2.07557714935415	0.50514616768862
C	-2.31712633923522	3.78487170694632	-0.03289478173400
C	-1.88343568292757	-1.12929115601026	-5.72063231770377
C	-4.36692114447771	1.79002910732381	-5.56460164253025
C	-3.98985171199191	-0.47286201603059	-2.71377910186599
C	-1.70006993999469	-5.20960110420247	-2.57394783616293
C	2.83910839403793	-2.24009604400955	-2.91921084500674
C	-3.21210688190210	-6.67718145384254	0.55805157843251
C	-5.04420988119321	-0.56404695645948	0.73406883237164
C	-6.37547219211320	-4.08263297135741	1.16412371737508
H	2.60302966859786	1.99987026774543	-2.63129810570640
H	1.49154552030723	0.62941410131999	-2.79771529526078
H	1.80680232777195	1.68743945049142	-4.18794083199481
H	0.29753212351109	-1.66833118240498	1.50010501915913
H	-0.84660268581483	-2.59475779692381	0.49561934710607
H	0.89625212235770	-2.78722470924768	0.24265616781948
H	-2.35809013861139	4.76852810809102	0.43912072744687
H	-1.57589698613496	3.80218588373655	-0.83284890073604
H	-3.29364943770712	3.55861144950591	-0.46329349662708
H	-1.49929617671902	-1.94695375569078	-6.33193161226865
H	-2.72940667378602	-1.49124046455629	-5.13729284388396
H	-2.21083850017390	-0.31368695996150	-6.36808004414463
H	-5.06984219497165	2.22109536938415	-6.27978767274382
H	-4.27540426027067	0.72180368164302	-5.76370210420077
H	-4.75786567076522	1.92480461026065	-4.55529670138004
H	-3.13054669382037	-1.03950394909504	-3.06631020014784
H	-4.46485968569882	-1.02497097251534	-1.90089819889461
H	-4.70076934710799	-0.34688137407672	-3.53270823026077
H	-2.47752864374935	-5.96551178533817	-2.69624700437910
H	-0.97203919597323	-5.30724922690956	-3.37969847486828
H	-1.21112789638241	-5.34632500165400	-1.60877663323365
H	2.74913774077254	-1.62555234235300	-2.02202431177974
H	3.8442583777369	-2.66390014500710	-2.96028133134661
H	2.69066287921055	-1.60127474721068	-3.79147235563666
H	-4.28586347081544	-6.50692694303872	0.64178896574579
H	-2.98739921971962	-6.95998689235672	-0.47147430616002

H	-2.93280702948057	-7.50330119640378	1.21464849828224
H	-4.98778207885476	0.28158447490792	0.04606028953535
H	-5.70817072047070	-1.32469677167788	0.31768442416539
H	-5.43475854563724	-0.22084492846178	1.69309219039673
H	-6.15633207891479	-3.16478868848858	1.71317281291755
H	-7.44420466712045	-4.29007318940110	1.24380808570932
H	-5.82388609549608	-4.90099451327686	1.62910827260467

**[Hg<sub>4</sub>(SMe)<sub>12</sub>]<sup>4-</sup>- $\alpha$**

Hg	-2.36427047969126	1.14481482895138	0.43161471250104
Hg	-2.07749050523275	-2.64072992770718	-1.55003653135851
Hg	-2.17300893411990	0.50310231680434	-4.05917728145523
Hg	-4.79505724627367	-3.94646400680246	0.25631900356187
S	-0.44473333523873	2.52981022562863	1.37474482238020
S	-2.55462041662651	2.03351643112303	-2.06959278752110
S	-1.06796805613946	-0.94709020770156	0.09037773746995
S	-4.54067515582906	1.75929978187045	1.31234661154778
S	-4.46269870938813	-2.55820785231868	-2.02673971085401
S	-0.76610315626665	-4.67057503902565	-1.17684699717545
S	-0.92924775775312	-1.66404873168524	-3.74801328062706
S	-4.05320442441642	-6.19754778467512	-0.42012767913072
S	-3.69592792519385	-2.48370395923335	1.88426034001537
S	-7.29532116177677	-3.89825493846874	0.51437881431992
S	-0.83844074422517	1.98165942762413	-5.60444477979602
S	-4.37714255470984	0.05822449725225	-5.12482581236149
C	-1.29633528266833	4.12397425777240	1.63757231483916
C	-4.72597073057372	3.42103447700347	0.57440349734976
C	-2.06533323507822	3.32881949828805	-5.72183433741504
C	-3.83422612986284	0.00972797435737	-6.86946966385160
C	-1.91744536403607	-2.70627713206599	-4.87564488995434
C	0.89200213706218	-3.90202585786707	-1.15415076897577
C	-5.59265285279471	-7.15951379730731	-0.17744584944991
C	-7.41961753916116	-4.81572162686856	2.08980899267807
C	-5.13967255853513	-1.55303387551442	2.50667996546211
C	-1.17960141158922	3.22939855445611	-2.16855171597529
C	0.25293571067791	-0.20293238376607	-0.92596116639721
C	-4.88783806727207	-0.89422244920933	-1.42155338524466
H	-0.61797104953124	4.83188276480386	2.11831979693038
H	-1.62065975705702	4.54638258180627	0.68446237977435
H	-2.17279776942874	3.99489263423175	2.27392387668144
H	-5.77872024966582	3.70543764698863	0.62984159442094
H	-4.13433575220830	4.16621748516280	1.10538519042402
H	-4.41378101012016	3.40433987691800	-0.47094553024279
H	-1.70947447759935	4.09898666999082	-6.40936310342690
H	-3.02129052179361	2.94585142186313	-6.08438717490713
H	-2.23185175791343	3.78210908821924	-4.74228830570315
H	-3.31103674824236	-0.92470393689672	-7.08343586424619
H	-4.70504795036234	0.07746915575050	-7.52505064271511
H	-3.15610410193989	0.83562364854430	-7.08841140104540
H	-1.74428451664017	-3.75598545338566	-4.63003474801746
H	-2.97597818373255	-2.46866354473001	-4.75693601282610
H	-1.61879368066456	-2.52455129209375	-5.90952659589630

H	0.98182019860391	-3.20732710832136	-0.31708593251648
H	1.64740302676675	-4.68310179093646	-1.04515998296643
H	1.07670367872693	-3.35685958058130	-2.08149891987599
H	-6.46717385273798	-6.53492376485495	-0.36649579324673
H	-5.60054714794181	-8.00598382047162	-0.86688571746018
H	-5.65695901033245	-7.54580859010590	0.84122791077210
H	-6.83376831379720	-4.32873392637422	2.87163033237929
H	-8.46191419200969	-4.85282960655425	2.41320886728685
H	-7.05683564083581	-5.83853513127822	1.97697223459669
H	-5.55841221203913	-0.93125828713384	1.71659068993314
H	-5.91716443555301	-2.22175014453199	2.87677264733215
H	-4.81026152182815	-0.90031831921536	3.31784929221009
H	-1.57608787579173	4.24604281642360	-2.12225873231168
H	-0.50539564631637	3.07424701512082	-1.32324746711159
H	-0.64678791570893	3.09113212197529	-3.11190266588233
H	-0.18452459481729	0.32438035951245	-1.77528020488125
H	0.81248023679492	0.50873330676981	-0.31642367544507
H	0.91902564610807	-0.98698119353459	-1.28720450334534
H	-4.49323056041562	-0.74904658764056	-0.41649277425754
H	-4.47229966206984	-0.13842111382450	-2.09006091347375
H	-5.97625754119340	-0.80159992253092	-1.39686378552232

**[Hg(Cys)<sub>2</sub>]<sup>-1</sup>**

Hg	-0.32584291702576	0.28210765506501	-0.66771940872817
S	-0.02910994631018	0.82487480255772	-2.91848291002342
S	-0.99781414787842	-0.78211069119653	1.30723506144050
O	2.71888467036932	4.24028437117704	-0.70322767932050
O	3.77607573787458	3.53470655583151	-2.56506779385168
O	-1.70540819190789	2.72243595867956	0.08483190719089
O	-0.12183668750883	3.26642316172141	1.60666345837885
N	1.57151518431963	1.76799180250853	-0.31238177996864
N	-3.12949703620746	1.31736213060594	1.72420890681519
C	0.97627619393867	2.32395586973376	-2.61685916737014
C	-0.92602465394143	0.53638164522128	2.56832532087593
C	2.11674255426423	2.11452320167208	-1.62270089143745
C	2.95550538425474	3.41115695311775	-1.61759614614297
C	-1.80997178808523	1.74498790606171	2.25736720538309
C	-1.15040133810547	2.67578090406608	1.21965215397735
H	-3.25834309975711	1.84696112860797	0.84580520310419
H	-3.90533631728641	1.48757942550987	2.36297399284743
H	1.38958899339941	2.61993399511197	-3.58265923132709
H	0.32394298145323	3.12326325936280	-2.25239951103617
H	-1.25661610422811	0.05793186298286	3.49334838946729
H	0.09355477633557	0.89450103221505	2.71000075856622
H	2.74312163085367	1.29141530766231	-1.97469686168916
H	-3.09924488716929	0.31792429654433	1.47578965362095
H	-1.97751173350311	2.31213575972626	3.17323120318988
H	1.24203708770375	2.62064429565066	0.15082956501689
H	2.30470365414786	1.38323740980307	0.27876860102071

**[Hg(Cys)<sub>2</sub>]<sup>-2</sup>**

Hg 0.52311 3.39704 5.28669  
 S 1.14106 3.37658 3.01575  
 S -0.03747 4.01260 7.48276  
 O -0.76040 -1.08504 3.57979  
 O -1.25467 -0.38469 1.49558  
 O -0.02912 0.05246 7.08585  
 O -0.24394 0.86705 9.17449  
 N -0.92272 1.49604 4.55904  
 N 1.95546 1.67757 6.43824  
 C 0.30017 0.80259 8.04392  
 C 0.70925 1.62211 2.73471  
 C -0.72468 1.26339 3.13330  
 C 1.31384 3.11862 8.33311  
 C 1.54168 1.69431 7.84022  
 C -0.94839 -0.20169 2.70473  
 H -0.59540 0.68662 5.09256  
 H -1.91308 1.59524 4.76508  
 H 1.71655 0.76252 6.06055  
 H 2.95776 1.81988 6.34701  
 H 0.84248 1.42946 1.66803  
 H 1.40500 0.98366 3.28894  
 H -1.40776 1.90441 2.57106  
 H 2.24000 3.69091 8.23168  
 H 1.04104 3.08239 9.38834  
 H 2.32373 1.26727 8.48539  
 H -0.59540 0.68662 5.09256  
 H -1.91308 1.59524 4.76508

**[Hg(Cys)<sub>4</sub>]<sup>2-</sup>**

Hg 0.12436498377521 -0.08728906197924 1.71985122508755  
 S 0.19954766521099 2.09694694360738 2.97110600558000  
 S 2.19592709932577 -0.17889744527873 0.29775648088502  
 S -0.18953884830067 -2.14382317142838 3.11164255594681  
 S -1.76939629811859 -0.03717099484438 0.05445936987504  
 O 0.01656544390701 5.97795837332335 3.12573170960213  
 O -0.25084707680996 5.16501655839776 1.03914636130481  
 O -0.54833262291564 -4.68626782167906 0.54906322495843  
 O -4.23910438268406 2.85881919582636 -0.55682996397288  
 O -0.10154942834091 -5.90607790767942 2.39439449378472  
 O -3.56180444003214 1.97191701034019 -2.51868737162225  
 O 4.29471061302168 -3.43742308142266 -0.16387166352262  
 O 4.16298549569755 -2.23386450830270 -2.06843537992024  
 N 1.99561683133060 4.44097569200441 3.74708022259262  
 N -1.74540744303272 -4.64698139434763 3.93393374926348  
 N 1.79045854765251 -3.25136039269585 0.42932878517190  
 N -1.89113120574393 3.02852442015907 0.48060461578164  
 C -1.13851578442401 1.25133817211079 -1.07852616415119  
 C 3.68404059708203 -2.78293054705654 -1.05250728606332  
 C 0.32452795742400 5.24790146726121 2.15730469907728  
 C -1.89943813512158 2.55984935521275 -0.92592177809277  
 C -1.72844497674269 -2.76546394167031 2.33832463197523  
 C -1.83318294947732 -4.27042548324649 2.49842520531082

C	-0.71512754266650	-5.02466354578495	1.75245628971373
C	-3.37503422027644	2.44014381143273	-1.37520801828272
C	1.61925733475301	-1.27446613253748	-1.04560795640212
C	1.40464950352252	2.94262617773073	1.88521740734828
C	1.59307103450426	4.38449967102600	2.31808627558865
C	2.14907445426814	-2.69137023099322	-0.89428523378236
H	1.70266975721896	-3.33676904303452	-1.65758346811600
H	0.91673174497837	-3.82277716748736	0.42965245909165
H	2.60794109204441	-3.80949444860314	0.71873951047839
H	1.06384985191523	2.94723396645380	0.84955942251521
H	2.36092603227973	2.41460869519390	1.91122712864235
H	-1.27307638364515	0.92261691803277	-2.10997563059178
H	-0.06834430628421	1.40056085539632	-0.90578152108060
H	-1.43041750246230	3.33508981226902	-1.53962036558375
H	-1.24318260703792	3.82316733030005	0.66772611652367
H	-2.87102265882055	3.30282702517489	0.66693178726512
H	1.98556260653863	-0.89312333788915	-1.99944249310466
H	0.52499937561548	-1.27371627695198	-1.06706489271887
H	-1.72663304031933	-2.54839726706189	1.27043982900774
H	-2.59667354550938	-2.27627576773134	2.78822878710970
H	-2.79563511547120	-4.62772711980435	2.12336278113206
H	-1.27761591248446	-5.56288547266941	3.97675600929527
H	-1.14182533834019	-3.96978329113076	4.41979184468499
H	3.00514375395766	4.41907951959760	3.88819786801489
H	-1.65750099916728	2.25242860258009	1.11680512116426
H	-2.64993774874325	-4.68225991737210	4.40317499923614
H	1.68660200043790	-2.48416657816348	1.10926317132592
H	2.38910715021996	4.85299828605265	1.73357321460711
H	1.59305876305946	5.30506457167693	4.13666637940870
H	1.56895760279398	3.64351294504566	4.24053627787572

## 6. NPA analysis of the Hg(CysSerGlyCysLys) complex

Natural Population					
Natural -----					
Atom No	Charge	Core	Valence	Rydberg	Total
-----					
Hg 1	1.06183	67.99542	10.72758	0.21516	78.93817
S 2	-0.44007	9.99936	6.29160	0.14911	16.44007
S 3	-0.43215	9.99936	6.28431	0.14848	16.43215
O 4	-0.64211	1.99955	6.55322	0.08935	8.64211
O 5	-0.63313	1.99955	6.54408	0.08950	8.63313
O 6	-0.66806	1.99954	6.57454	0.09398	8.66806
O 7	-0.72268	1.99967	6.63534	0.08767	8.72268
O 8	-0.67155	1.99952	6.58205	0.08999	8.67155
O 9	-0.65672	1.99955	6.56580	0.09137	8.65672
N 10	-0.56393	1.99912	5.48461	0.08020	7.56393
N 11	-0.61915	1.99912	5.53597	0.08407	7.61915
N 12	-0.56526	1.99911	5.48922	0.07693	7.56526
N 13	-0.82570	1.99943	5.74028	0.08600	7.82570
N 14	-0.59349	1.99913	5.51382	0.08053	7.59349

N 15	-0.86233	1.99944	5.77320	0.08969	7.86233
N 16	-0.77978	1.99923	5.70131	0.07924	7.77978
C 17	-0.16409	1.99895	4.10071	0.06443	6.16409
C 18	-0.15434	1.99895	4.09032	0.06508	6.15434
C 19	0.63271	1.99918	3.29417	0.07394	5.36729
C 20	-0.51185	1.99908	4.44007	0.07269	6.51185
C 21	0.63654	1.99909	3.28592	0.07845	5.36346
C 22	-0.15222	1.99897	4.09015	0.06310	6.15222
C 23	0.65563	1.99914	3.26072	0.08451	5.34437
C 24	-0.05088	1.99905	3.99131	0.06052	6.05088
C 25	0.63448	1.99911	3.27963	0.08678	5.36552
C 26	0.64081	1.99919	3.28436	0.07564	5.35919
C 27	-0.15363	1.99896	4.08843	0.06623	6.15363
C 28	-0.51166	1.99908	4.43603	0.07655	6.51166
C 29	-0.30760	1.99903	4.25159	0.05698	6.30760
C 30	-0.37911	1.99914	4.32522	0.05475	6.37911
C 31	-0.38995	1.99918	4.33257	0.05820	6.38995
C 32	-0.40162	1.99918	4.34382	0.05862	6.40162
C 33	-0.19672	1.99919	4.14098	0.05654	6.19672
H 34	0.45496	0.00000	0.53775	0.00730	0.54504
H 35	0.24336	0.00000	0.75061	0.00604	0.75664
H 36	0.43769	0.00000	0.55746	0.00485	0.56231
H 37	0.42502	0.00000	0.56902	0.00596	0.57498
H 38	0.17945	0.00000	0.81470	0.00585	0.82055
H 39	0.19981	0.00000	0.79366	0.00653	0.80019
H 40	0.23920	0.00000	0.75398	0.00682	0.76080
H 41	0.20730	0.00000	0.78679	0.00591	0.79270
H 42	0.43210	0.00000	0.56341	0.00449	0.56790
H 43	0.23402	0.00000	0.75952	0.00647	0.76598
H 44	0.22817	0.00000	0.76537	0.00646	0.77183
H 45	0.36781	0.00000	0.62652	0.00567	0.63219
H 46	0.23236	0.00000	0.76097	0.00666	0.76764
H 47	0.23316	0.00000	0.75879	0.00805	0.76684
H 48	0.36622	0.00000	0.62873	0.00505	0.63378
H 49	0.35864	0.00000	0.63590	0.00546	0.64136
H 50	0.16633	0.00000	0.82678	0.00690	0.83367
H 51	0.17584	0.00000	0.81740	0.00676	0.82416
H 52	0.20711	0.00000	0.78668	0.00620	0.79289
H 53	0.19186	0.00000	0.80206	0.00608	0.80814
H 54	0.19506	0.00000	0.79854	0.00640	0.80494
H 55	0.21369	0.00000	0.78003	0.00628	0.78631
H 56	0.21178	0.00000	0.78220	0.00603	0.78822
H 57	0.21260	0.00000	0.78150	0.00590	0.78740
H 58	0.48946	0.00000	0.50507	0.00547	0.51054
H 59	0.19158	0.00000	0.80222	0.00620	0.80842
H 60	0.22423	0.00000	0.77036	0.00541	0.77577
H 61	0.24415	0.00000	0.74992	0.00594	0.75585
H 62	0.42169	0.00000	0.57458	0.00373	0.57831
H 63	0.42500	0.00000	0.57041	0.00458	0.57500
H 64	0.37815	0.00000	0.61686	0.00500	0.62185

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\* Total \* 0.00000 147.97057 191.06072 2.96872 342.00000

### Natural Population

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Effective Core      60.00000
Core                87.97057 ( 99.9666% of  88)
Valence            191.06072 ( 98.4849% of 194)
Natural Minimal Basis 339.03128 ( 99.1320% of 342)
Natural Rydberg Basis  2.96872 (  0.8680% of 342)
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### Atom No      Natural Electron Configuration

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-----
Hg 1  [core]6s( 0.98)5d( 9.75)6p( 0.08)5f( 0.09)6d( 0.03)7p( 0.01)
S 2  [core]3s( 1.76)3p( 4.53)4s( 0.01)3d( 0.10)4p( 0.03)4f( 0.01)
S 3  [core]3s( 1.76)3p( 4.52)4s( 0.01)3d( 0.10)4p( 0.03)4f( 0.01)
O 4  [core]2s( 1.69)2p( 4.87)3s( 0.01)3p( 0.03)3d( 0.04)
O 5  [core]2s( 1.69)2p( 4.85)3s( 0.01)3p( 0.03)3d( 0.04)
O 6  [core]2s( 1.70)2p( 4.88)3s( 0.01)3p( 0.04)3d( 0.04)
O 7  [core]2s( 1.68)2p( 4.96)3s( 0.01)3p( 0.04)3d( 0.04)
O 8  [core]2s( 1.69)2p( 4.89)3s( 0.01)3p( 0.03)3d( 0.04)
O 9  [core]2s( 1.70)2p( 4.87)3s( 0.01)3p( 0.04)3d( 0.04)
N 10 [core]2s( 1.26)2p( 4.22)3s( 0.01)3p( 0.03)3d( 0.04)
N 11 [core]2s( 1.28)2p( 4.26)3s( 0.01)3p( 0.03)3d( 0.04)
N 12 [core]2s( 1.27)2p( 4.22)3p( 0.03)3d( 0.04)
N 13 [core]2s( 1.43)2p( 4.31)3p( 0.03)3d( 0.04)
N 14 [core]2s( 1.28)2p( 4.24)3s( 0.01)3p( 0.03)3d( 0.04)
N 15 [core]2s( 1.43)2p( 4.34)3p( 0.04)3d( 0.04)
N 16 [core]2s( 1.33)2p( 4.37)3p( 0.03)3d( 0.04)
C 17 [core]2s( 1.02)2p( 3.08)3p( 0.02)3d( 0.02)
C 18 [core]2s( 1.00)2p( 3.09)3p( 0.03)3d( 0.02)
C 19 [core]2s( 0.83)2p( 2.47)3s( 0.01)3p( 0.04)3d( 0.02)
C 20 [core]2s( 1.13)2p( 3.31)3p( 0.02)3d( 0.04)
C 21 [core]2s( 0.81)2p( 2.47)3s( 0.01)3p( 0.04)3d( 0.02)4f( 0.01)
C 22 [core]2s( 1.00)2p( 3.09)3p( 0.02)3d( 0.02)
C 23 [core]2s( 0.82)2p( 2.44)3s( 0.01)3p( 0.04)3d( 0.02)4d( 0.01)
C 24 [core]2s( 1.03)2p( 2.96)3s( 0.01)3p( 0.02)3d( 0.03)
C 25 [core]2s( 0.83)2p( 2.45)3s( 0.01)3p( 0.04)3d( 0.02)4f( 0.01)
C 26 [core]2s( 0.82)2p( 2.46)3s( 0.01)3p( 0.04)3d( 0.02)
C 27 [core]2s( 1.01)2p( 3.08)3p( 0.02)3d( 0.03)
C 28 [core]2s( 1.12)2p( 3.32)3p( 0.02)3d( 0.04)
C 29 [core]2s( 1.06)2p( 3.19)3p( 0.02)3d( 0.03)
C 30 [core]2s( 1.06)2p( 3.27)3p( 0.02)3d( 0.03)
C 31 [core]2s( 1.04)2p( 3.29)3p( 0.02)3d( 0.03)
C 32 [core]2s( 1.05)2p( 3.29)3p( 0.02)3d( 0.03)
C 33 [core]2s( 1.03)2p( 3.11)3p( 0.02)3d( 0.02)
H 34      1s( 0.54)
H 35      1s( 0.75)
H 36      1s( 0.56)
H 37      1s( 0.57)
H 38      1s( 0.81)
H 39      1s( 0.79)
H 40      1s( 0.75)

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H 41	1s( 0.79)
H 42	1s( 0.56)
H 43	1s( 0.76)
H 44	1s( 0.77)
H 45	1s( 0.63)
H 46	1s( 0.76)
H 47	1s( 0.76)
H 48	1s( 0.63)
H 49	1s( 0.64)
H 50	1s( 0.83)
H 51	1s( 0.82)
H 52	1s( 0.79)
H 53	1s( 0.80)
H 54	1s( 0.80)
H 55	1s( 0.78)
H 56	1s( 0.78)
H 57	1s( 0.78)
H 58	1s( 0.51)
H 59	1s( 0.80)
H 60	1s( 0.77)
H 61	1s( 0.75)
H 62	1s( 0.57)
H 63	1s( 0.57)
H 64	1s( 0.62)