

Hydrotropic solubilization of gold nanoparticles functionalized with proto-alkylthioporphyrazines

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Experimental Section

H₂OESPz was synthesized according to ref.¹ The dianionic form of the 2,3,7,8,12,13,17,18-*octakis*-ethylthio-5,10,15,20-(21*H*, 23*H*) porphyrazine was obtained as disodium salt (Na₂OESPz) by dissolving the free base (10⁻⁵ M) in chloroform and adding 0.5% v/v of NaOH 0.5 M in methanol. The color of the porphyrazine solution changed from deep blue to brilliant green, indicating that deprotonation of the tetra-aza macrocycle had occurred. The solvent was then removed with a nitrogen stream. Freshly prepared Na₂OESPz in 1 M NaOH/methanol was always used and directly added to the Au nanoparticles in water.

Au nanospheres of 40 nm diameter were prepared by the well established Turkevitch method,² that consists in the reduction of HAuCl₄ with trisodium citrate under stirring at reflux. In our case, 0.16 ml of 3.87 10⁻² M citrate solution were added dropwise to 50 ml of 2.5 10⁻⁴ M, in order to reach citrate/Au = 0.5 molar ratio³ and the reaction was allowed to proceed for 15'. The pH of as prepared Au nanoparticles was 5.5. The size of nanoparticles was checked by Dynamic Light Scattering with a Coulter Sub-Micron Particle Analyzer N4SD, equipped with a $\lambda = 632.8$ nm helium-neon laser and 90° detector. The autocorrelation function of the scattered light was analyzed by the SDP (Size Distribution Processor) procedure, based on the algorithm CONTIN.⁴

UV-visible spectra were measured with a Varian Cary 5 spectrophotometer.

Raman spectra were obtained by excitation with the 568.2 and 647.1 nm lines of a Kr⁺ laser (Coherent, Innova 300 C), and the 514.5 nm line of an Ar⁺ laser (Coherent, Innova 90). The back-scattered light from a slowly rotating NMR tube was collected and focused into a triple spectrometer (consisting of two Acton Research SpectraPro2300i working in the subtractive mode, and a SpectraPro 2500i in the final stage with a 1800 grooves/mm grating), equipped with a liquid-nitrogen cooled CCD detector. The wavenumbers were calibrated with various solvents (indene, carbon tetrachloride, chloroform) as standards.

References

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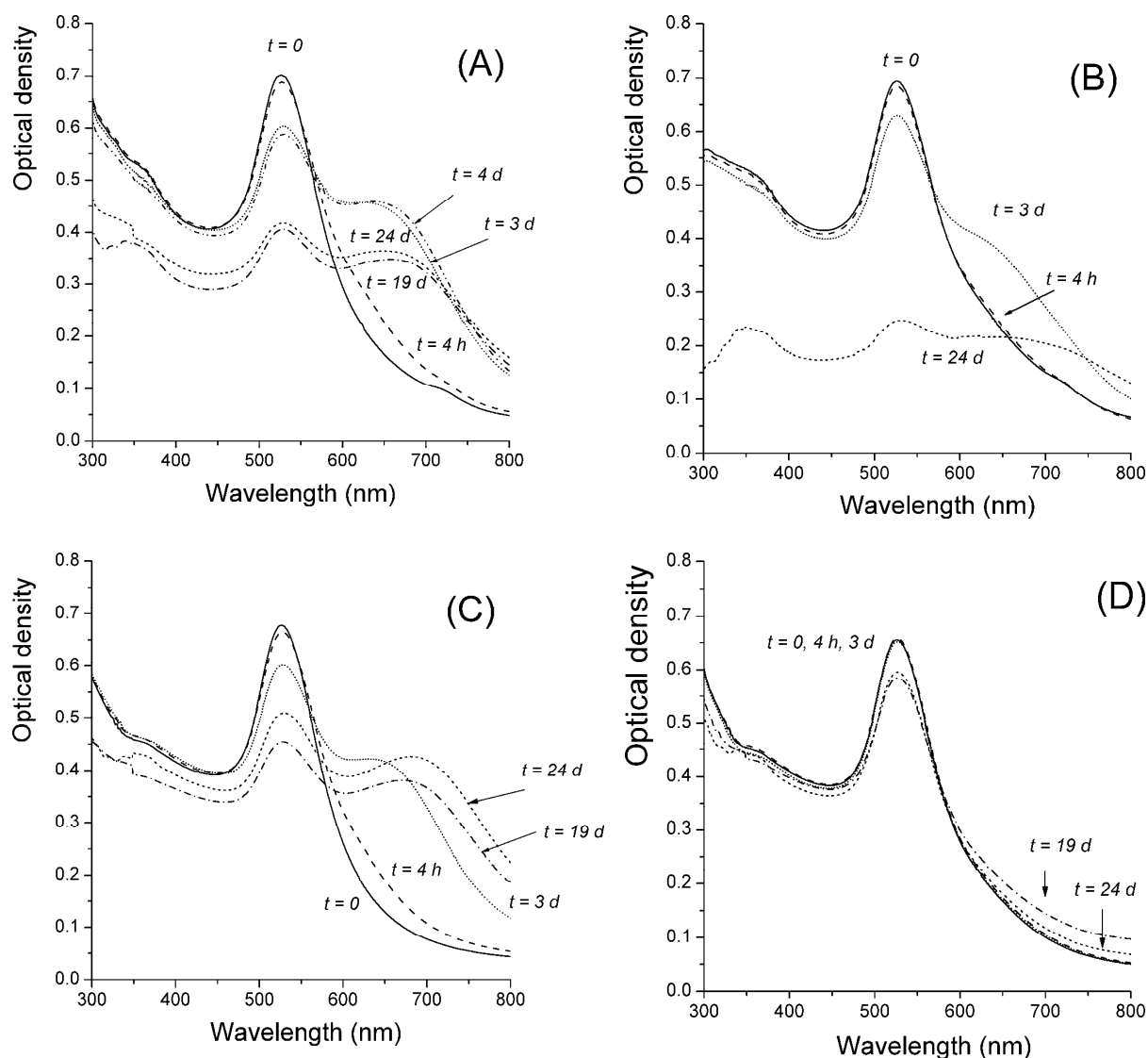
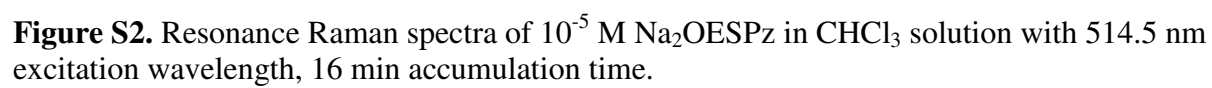


Figure S1. (A) Time-dependent absorption spectra of GNPs after the addition of 17% v/v NaOH 0.1 M in methanol containing Na₂OESPz (2×10^{-6} M final concentration), pH = 13. (B) Time-dependent absorption spectra of the same dispersion as (A) where the pH was immediately adjusted to 7 with citric acid (6.6 mM final concentration). (C) Time-dependent absorption spectra of GNPs after the addition of 17% v/v NaOH 0.1 M in methanol, pH = 13. (D) Time-dependent absorption spectra of the same dispersion as (C) where the pH was immediately adjusted to 7 with citric acid (6.6 mM final concentration).

Notes: The final spectra in (A) and (B) are those shown in Figure 1 in the manuscript. The spectra in (C) and (D) allow for a comparison between dispersions with and without Na₂OESPz.



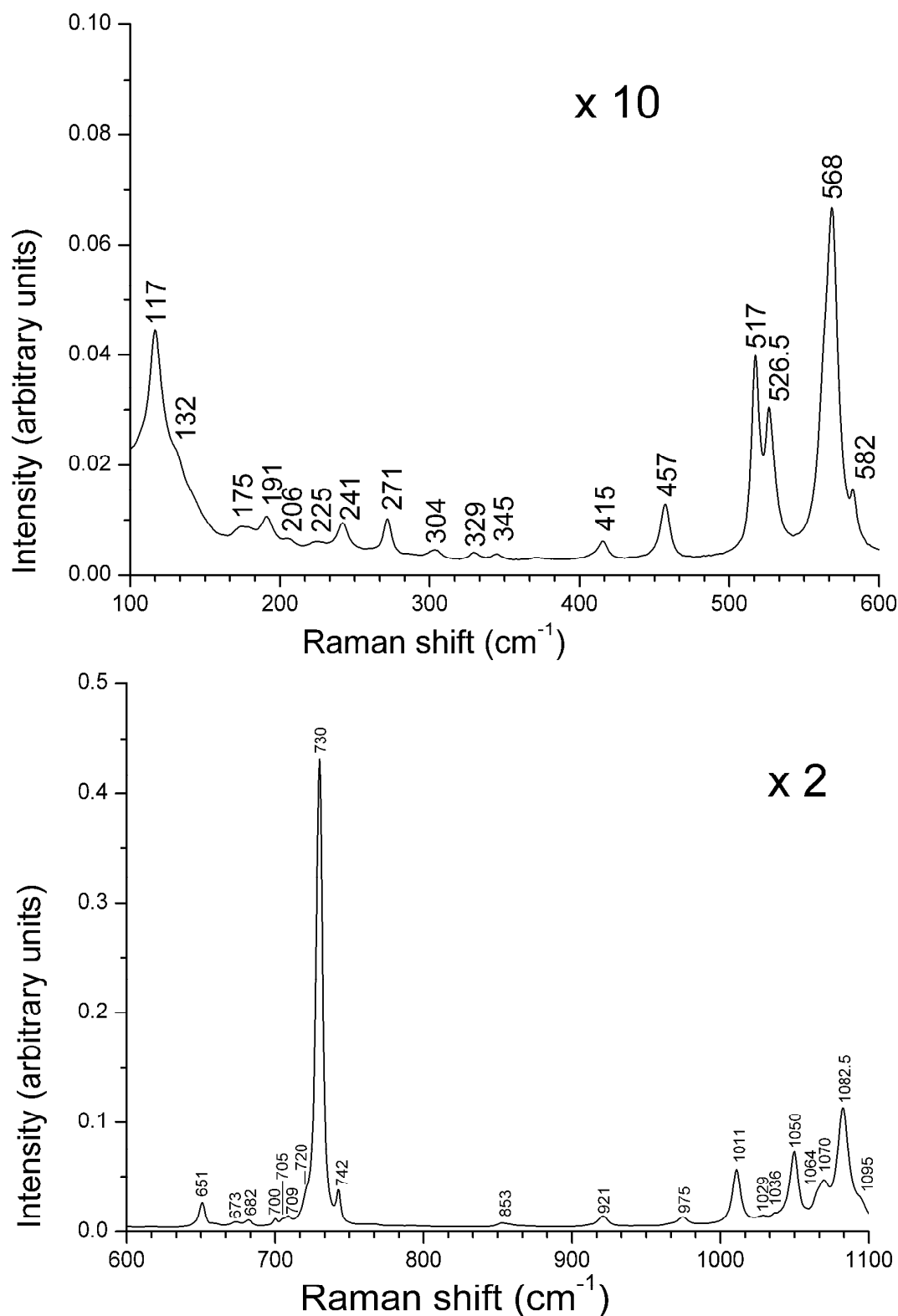


Figure S3. Fourier-Transform Raman spectrum of solid H_2OESPz with 1064 nm excitation in the range 100-600 cm^{-1} (top) and 600-1100 cm^{-1} (bottom). Raman spectra were collected using a FT-Raman RFS100 Bruker system equipped with a liquid-nitrogen cooled Ge detector. A c.w. Nd:YAG laser (1064 nm) was used as an excitation source. The scattered light was collected in backscattering geometry, spectral resolution 1 cm^{-1} . The power density at the sample was $3.2\text{W}/\text{cm}^2$. We checked the absence of sample overheating. The Raman scattered light was averaged over 512 scans. The spectra are corrected for the detector response and the ν^4 dependence.

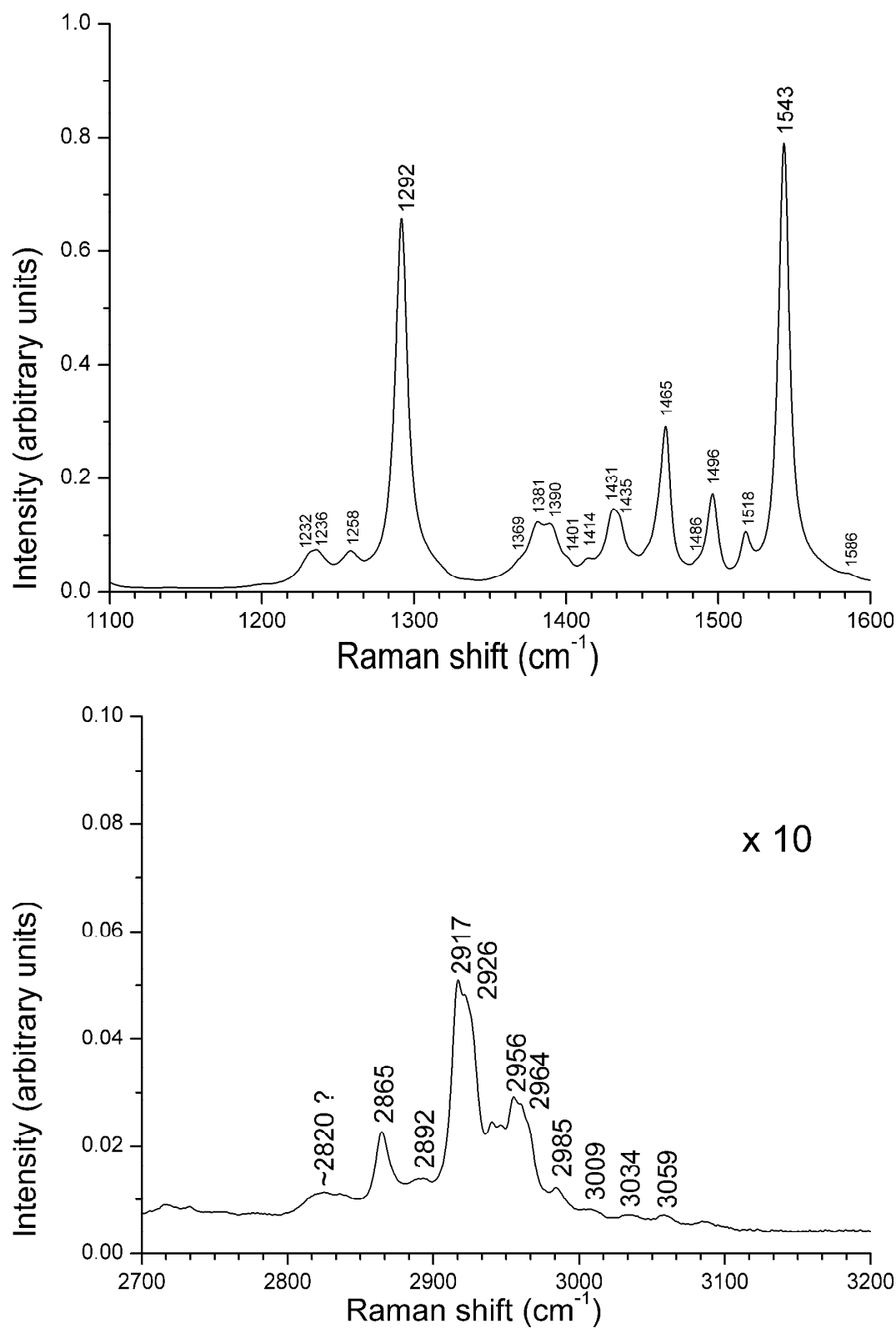


Figure S4. Fourier-Transform Raman spectrum of solid H_2OESPz with 1064 nm excitation in the range 1100-1600 cm^{-1} (top) and 2700-3200 cm^{-1} (bottom). Experimental conditions as in Figure S3.

Quantum Chemical Calculations. The ground state molecular structures of the model methylthioporphyrzine, H₂OMSPz, were fully optimized (without constraints) at the level of density functional theory (DFT) employing the standard GGA functional Becke–Perdew86 (BP86).^{1,2} The molecular structures were confirmed to be energy minima by calculating the harmonic vibrational frequencies. A selected number of structures (Figure S5), taken as representative of *uu*, *ud*, and combined, *uu* and *ud* (*u* = up, *d* = down) orientations of the vicinal methylthio groups, i. e. the methylthio groups residing on the same pyrrolic subunit, were theoretically explored for H₂OMSPz. The nearly degenerate **A** (*C*_{2h}) and **A** (*C*_{2v}) conformations, characterized by an *uu-uu-dd-dd* and *uu-dd-uu-dd* orientation of the vicinal methylthio groups, respectively, and by a substantially planar porphyrzineoctathiolate ring, are the preferred conformations in the “gas phase”. The particular stability of these structures can be traced to their capability to conjugate effective relief of the steric repulsions between the vicinal sulfur lone pairs and planarity of the porphyrzine core. The ground state equilibrium structures were computed with Turbomole V5.7³ employing the Karlsruhe triple- ζ valence quality basis sets augmented by one set of polarization functions (TZVP).⁴ In the BP86 DFT calculations, the resolution of the identity (density fitting) approach was used to save computer time.⁵ Raman intensities were computed with the ADF-RESPONSE module, which is an extension of the Amsterdam Density Functional (ADF) program system.^{6–8} The ADF calculations were performed with the BP86 functional and a TZP basis set, which is an uncontracted triple- ζ STO basis set with one 3d polarization function for C, N, and S atoms, and one 2p for H.

References

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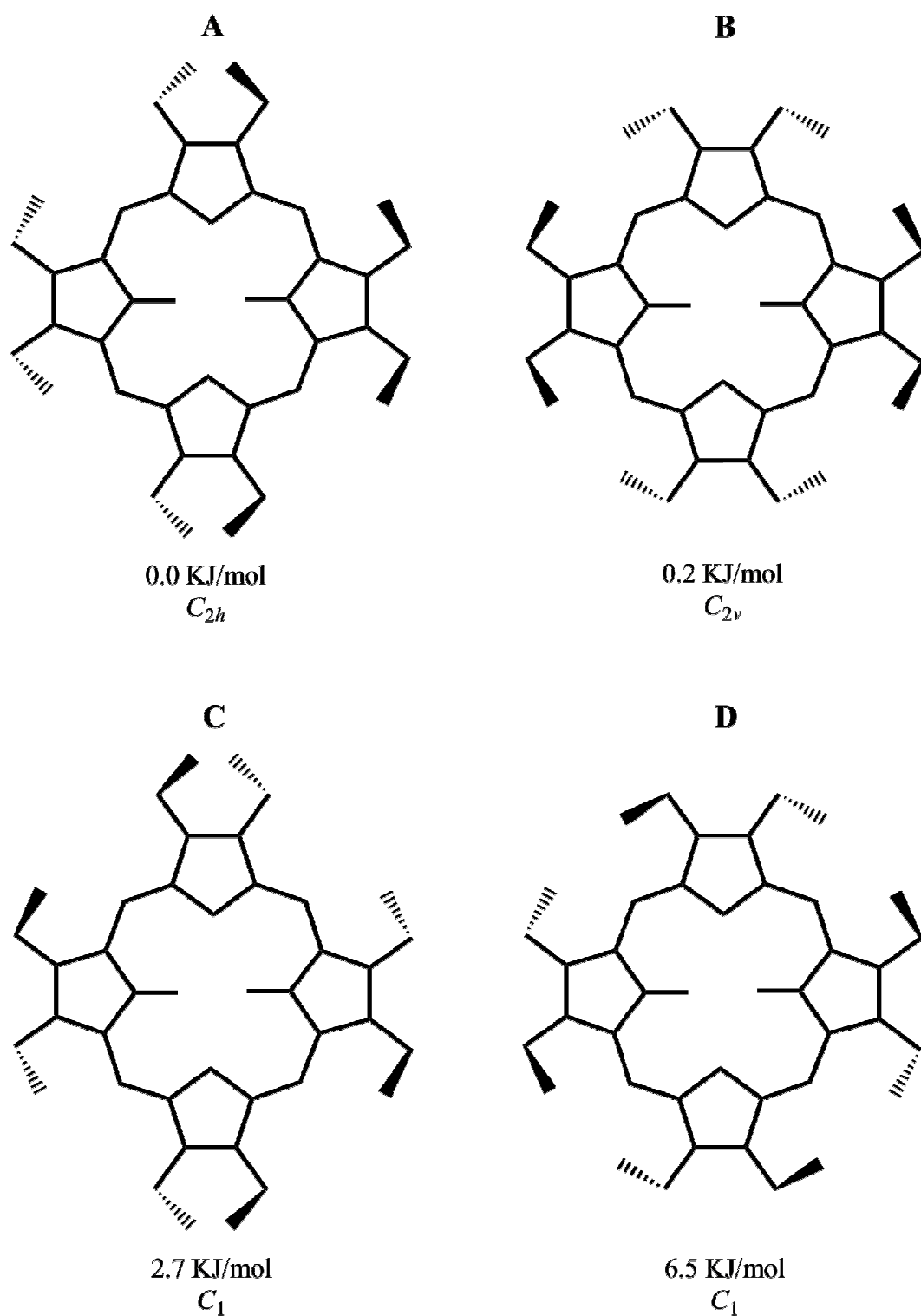


Figure S5. Schematic representation of the H₂OMSPz conformers considered in the DFT calculations. The energies refer to the DFT/BP86/TZVP optimized structures and are relative to the most stable A (C_{2h}) conformer. The energies include Zero-point Energy (ZPE) correction.

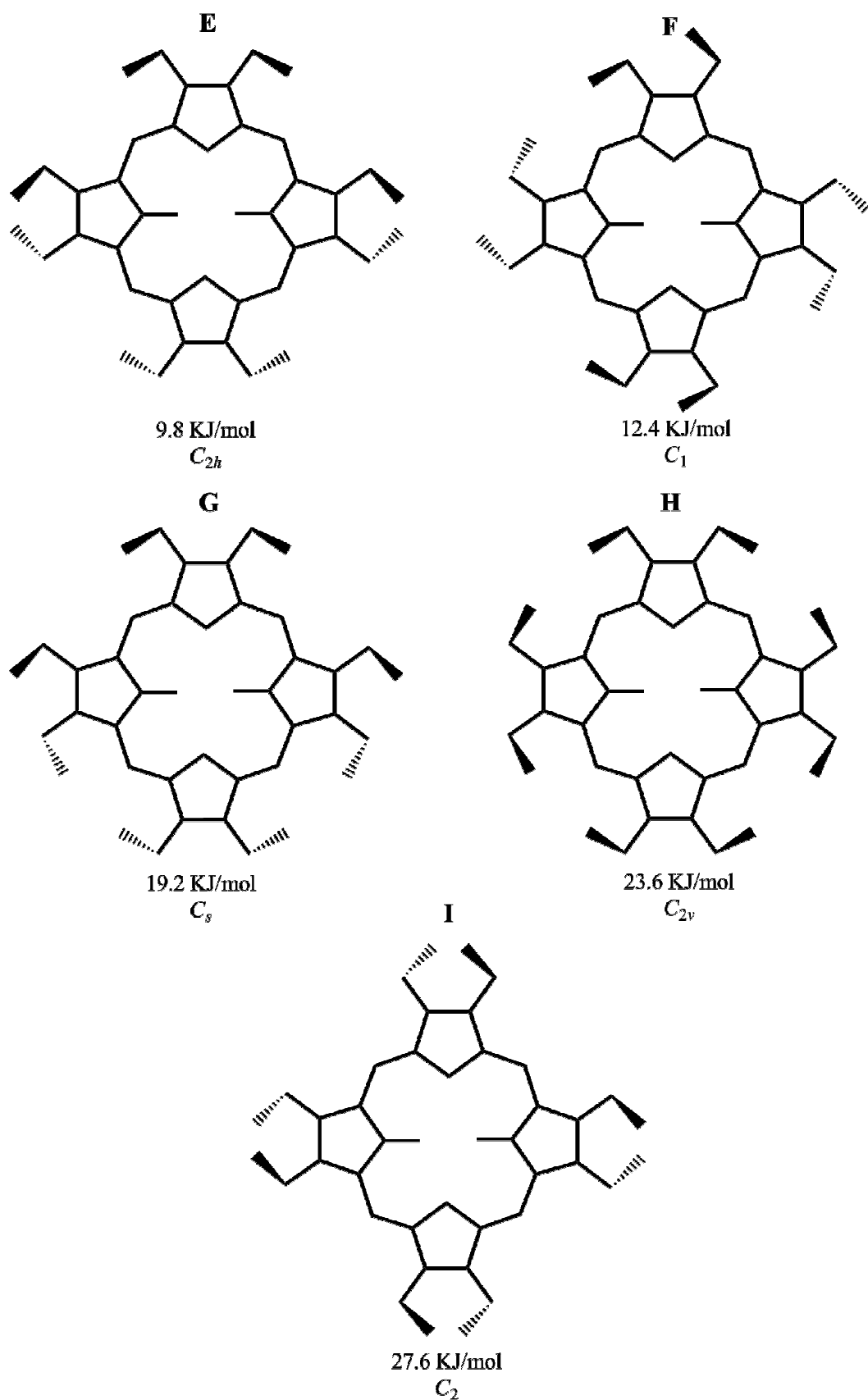


Figure S5(Continued). Schematic representation of the H₂OMSPz conformers considered in the DFT calculations. The energies refer to the DFT/BP86/TZVP optimized structures and relative to the most stable A (C_{2h}) conformer. The energies include Zero-point Energy (ZPE) correction.

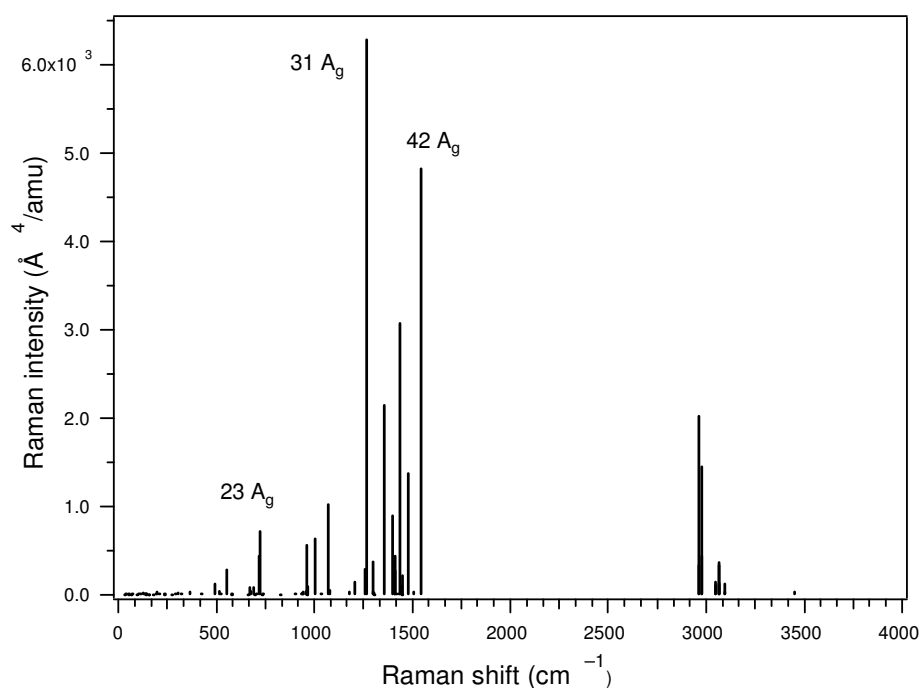


Figure S6. Raman spectrum (unscaled) computed in the gas-phase at DFT/BP86/TZP level of theory for the most stable **A** (C_{2h}) conformer of H_2OMSPz . The vibrational normal modes relevant to the interpretation of SERRS spectra of H_2OESPz functionalized GNPs in water solution are also indicated.

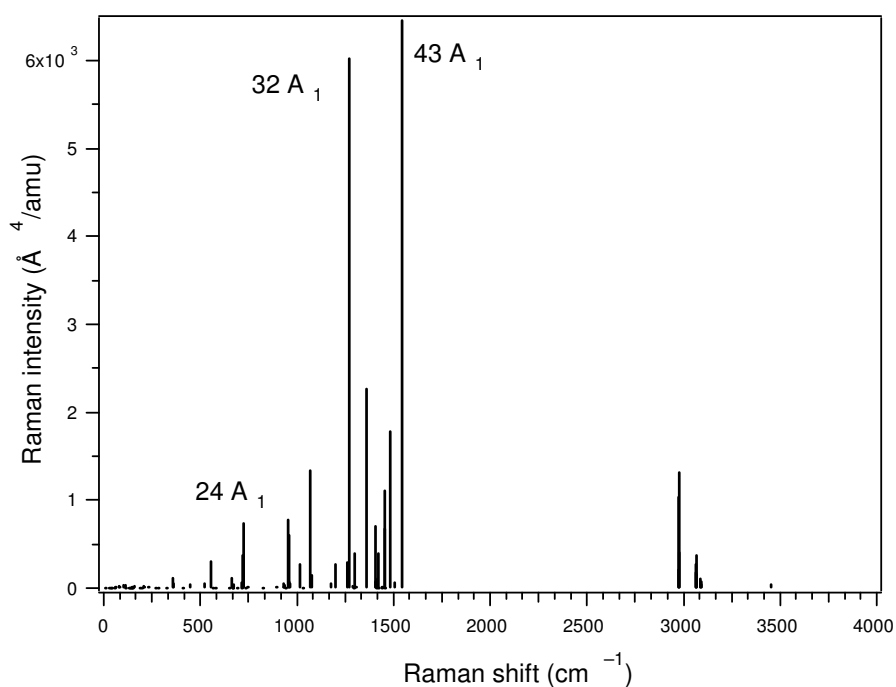


Figure S7. Raman spectrum (unscaled) computed in the gas-phase at DFT/BP86/TZP level of theory for the **B** (C_{2v}) conformer of H_2OMSPz . The vibrational normal modes relevant to the interpretation of SERRS spectra of H_2OESPz functionalized GNPs in water solution are also indicated

Cartesian coordinates of the DFT/BP86/TZVP optimized structures of the H₂OMSPz conformers.

A (*C*_{2h})

N	0.0000000	0.0000000	1.9166332
N	0.0000000	0.0000000	-1.9166332
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N	2.0245712	-0.0116068	0.0000000
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C	-1.0889937	0.0473852	-2.7420617
C	1.0889937	-0.0473852	2.7420617
C	1.0889937	-0.0473852	-2.7420617
C	-2.8014260	0.0824459	-1.1388679
C	-2.8014260	0.0824459	1.1388679
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C	2.8014260	-0.0824459	1.1388679
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C	-0.6898804	0.0193084	-4.1621411
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C	-4.1886362	0.1560819	0.6980823
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C	4.1886362	-0.1560819	0.6980823
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S	-1.8619239	-0.0154422	-5.4792873
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S	-5.6356997	0.3762925	-1.6709558
S	-5.6356997	0.3762925	1.6709558
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C	-1.2168725	-1.3899924	-6.5213726
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C	1.2168725	1.3899924	-6.5213726
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N	-2.3806188	0.0862482	-2.3919323
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H	-6.2066169	-0.4945045	-3.8004848
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H	6.2066169	0.4945045	-3.8004848
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H	-4.4157552	-0.3253828	-3.6817032
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H	1.0062915	0.0813958	0.0000000

B (C_{2v})

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H	3.5114200	4.2059920	-1.2966552

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C	-2.8010973	1.1364296	0.0693375
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C	2.8010023	-1.1364520	0.0694529
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C	-4.1890551	-0.6950119	-0.0652876
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H	1.7656446	-7.3983054	1.5542572
H	1.7664270	7.3986475	-1.5538465
H	-6.1313811	-3.7527761	-1.0731174
H	-1.7670798	-7.3982782	-1.5540363
H	6.1307660	3.7507732	-1.0785539
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H	-0.0950102	-6.8288492	-1.2215674
H	5.0229848	2.8085479	-2.1238989
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H	-1.1134041	5.9675290	2.4208700
H	4.3766371	-3.6791898	0.6648062
H	1.1151884	-5.9682246	2.4201750
H	1.1132948	5.9699649	-2.4200175
H	-4.3754993	-3.6768362	-0.6686145
H	-1.1153126	-5.9689164	-2.4201555
H	4.3730317	3.6717914	-0.6832523
H	0.9985043	-0.0007995	-0.0006689
H	-0.9986892	0.0004338	0.0002068

D (C_1)

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N	-0.0210722	-2.0105388	-0.0008615
N	1.9226684	-0.0199662	-0.0000669
N	0.0210242	2.0104590	-0.0022869
C	-2.7382496	1.1175728	-0.0514598
C	1.1068000	-2.8027456	0.0321625
C	2.7379842	-1.1174662	-0.0496042
C	-1.1068696	2.8024954	0.0294365
C	1.1651317	2.7790509	-0.0346073
C	2.7607194	1.0601963	0.0503074
C	-1.1652131	-2.7790455	-0.0340168
C	-2.7608491	-1.0600893	0.0487171
C	-4.1640534	0.7297936	-0.0642244
C	0.6518324	-4.1871337	0.0462956
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C	-0.6523657	4.1868025	0.0429042
C	0.7387849	4.1726847	-0.0495338
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C	-4.1778877	-0.6432375	0.0637676
S	-5.5622782	1.8026175	-0.0360289
S	1.6588054	-5.6324242	0.0185799
S	5.5608887	-1.8042161	-0.0361385
S	-1.6631035	5.6298784	0.0126901
S	1.7755052	5.5966999	-0.0215219
S	5.5974560	1.6878998	0.0401051
S	-1.7765350	-5.5963554	-0.0207648
S	-5.5973185	-1.6885112	0.0392184
C	3.0580891	5.1949707	-1.2842205
C	5.2706441	2.8267684	1.4535310
C	-3.0547757	-5.1963029	-1.2884457
C	-5.2705436	-2.8270540	1.4530223
C	5.2115755	-2.9379591	-1.4483436
C	-2.9348007	5.2620377	1.2968346
C	-5.2101404	2.9461920	-1.4395353
C	2.9456762	-5.2593755	1.2858462
N	-2.3675833	2.4037590	-0.0166019
N	2.3673131	-2.4038548	-0.0143640
N	2.4170471	2.3540777	0.0139278
N	-2.4172463	-2.3539713	0.0127063
H	3.7513490	6.0449059	-1.2631200
H	6.1052326	3.5389529	1.4522831
H	-3.7484220	-6.0459576	-1.2685369
H	-6.1058395	-3.5384193	1.4521964
H	6.0308667	-3.6676400	-1.4447895
H	-3.6125892	6.1244586	1.2795245
H	-6.0306929	3.6744434	-1.4336514
H	3.6215343	-6.1232379	1.2653089
H	3.5815896	4.2693942	-1.0292619
H	5.2714447	2.2675400	2.3963297
H	-3.5788344	-4.2702310	-1.0363236
H	-5.2704045	-2.2676640	2.3957421

H	5.2253959	-2.3803919	-2.3920073
H	-3.4792725	4.3449091	1.0554319
H	-5.2202609	2.3946579	-2.3867869
H	3.4886656	-4.3442941	1.0337350
H	2.5978371	5.1249676	-2.2765016
H	4.3237604	3.3561091	1.3122572
H	-2.5911612	-5.1277496	-2.2792538
H	-4.3242388	-3.3573362	1.3116196
H	4.2534270	-3.4468250	-1.3076960
H	-2.4619271	5.1902328	2.2830383
H	-4.2531539	3.4553944	-1.2924656
H	2.4840839	-5.1816012	2.2769155
H	-0.0103422	-0.9885893	-0.0010037
H	0.0107983	0.9884770	-0.0013820

E (C_{2h})

N	-1.9383703	0.0477228	0.0000000
N	1.9383703	-0.0477228	0.0000000
N	0.0000000	0.0000000	2.0017412
N	0.0000000	0.0000000	-2.0017412
C	-2.7636603	0.1073697	-1.0918617
C	-2.7636603	0.1073697	1.0918617
C	2.7636603	-0.1073697	-1.0918617
C	2.7636603	-0.1073697	1.0918617
C	-1.1351122	0.0600807	2.7796963
C	-1.1351122	0.0600807	-2.7796963
C	1.1351122	-0.0600807	2.7796963
C	1.1351122	-0.0600807	-2.7796963
C	-4.1830150	0.1638057	-0.6904489
C	-4.1830150	0.1638057	0.6904489
C	4.1830150	-0.1638057	-0.6904489
C	4.1830150	-0.1638057	0.6904489
C	-0.6968438	0.0250059	4.1692210
C	-0.6968438	0.0250059	-4.1692210
C	0.6968438	-0.0250059	4.1692210
C	0.6968438	-0.0250059	-4.1692210
N	-2.3941353	0.1072447	-2.3782857
N	-2.3941353	0.1072447	2.3782857
N	2.3941353	-0.1072447	-2.3782857
N	2.3941353	-0.1072447	2.3782857
S	1.8576914	-0.0249326	-5.4978548
S	1.8576914	-0.0249326	5.4978548
S	-1.8576914	0.0249326	-5.4978548
S	-1.8576914	0.0249326	5.4978548
S	-5.6180209	0.3833633	-1.6844595
S	-5.6180209	0.3833633	1.6844595
S	5.6180209	-0.3833633	-1.6844595
S	5.6180209	-0.3833633	1.6844595
C	-1.2469231	-1.3770399	-6.5239641
C	-1.2469231	-1.3770399	6.5239641
C	1.2469231	1.3770399	-6.5239641
C	1.2469231	1.3770399	6.5239641

C	-5.3260505	-0.7189910	3.1321084
C	-5.3260505	-0.7189910	-3.1321084
C	5.3260505	0.7189910	3.1321084
C	5.3260505	0.7189910	-3.1321084
H	0.0000000	0.0000000	0.9801486
H	0.0000000	0.0000000	-0.9801486
H	1.8998561	1.3997620	7.4049542
H	1.8998561	1.3997620	-7.4049542
H	-1.8998561	-1.3997620	7.4049542
H	-1.8998561	-1.3997620	-7.4049542
H	1.3430962	2.3160447	5.9675733
H	1.3430962	2.3160447	-5.9675733
H	-1.3430962	-2.3160447	5.9675733
H	-1.3430962	-2.3160447	-5.9675733
H	0.2046501	1.2309147	6.8333578
H	0.2046501	1.2309147	-6.8333578
H	-0.2046501	-1.2309147	6.8333578
H	-0.2046501	-1.2309147	-6.8333578
H	6.2078236	0.5830413	3.7708197
H	6.2078236	0.5830413	-3.7708197
H	-6.2078236	-0.5830413	3.7708197
H	-6.2078236	-0.5830413	-3.7708197
H	5.2698929	1.7638567	2.8046037
H	5.2698929	1.7638567	-2.8046037
H	-5.2698929	-1.7638567	2.8046037
H	-5.2698929	-1.7638567	-2.8046037
H	4.4163436	0.4274294	3.6633317
H	4.4163436	0.4274294	-3.6633317
H	-4.4163436	-0.4274294	3.6633317
H	-4.4163436	-0.4274294	-3.6633317

F (C₁)

N	-1.8201969	-0.8060918	0.0509845
N	1.6397724	0.8605377	0.0099483
N	-0.9467235	1.8544849	-0.0016012
N	0.7676227	-1.7864986	-0.0414045
C	-2.1101030	-2.1453523	0.0458949
C	-3.0276353	-0.1713138	0.0243298
C	2.8564034	0.2325612	0.0230555
C	1.9169814	2.1952594	-0.0078510
C	-2.3079133	2.0590585	0.0337238
C	0.0804656	-2.9782971	0.0118435
C	-0.2644080	3.0524454	-0.0232576
C	2.1287394	-1.9981225	-0.0573572
C	-3.5668712	-2.3907134	0.0228849
C	-4.1506919	-1.1372922	0.0119509
C	3.9707327	1.1980545	0.0444710
C	3.3788468	2.4456493	0.0142535
C	-2.5219246	3.5006472	0.0282071
C	1.0776730	-4.0438542	0.0024987
C	-1.2658095	4.1132014	-0.0029025

C	2.3351850	-3.4411599	-0.0509970
N	-1.2296154	-3.1545317	0.0415328
N	-3.2616054	1.1447438	0.0326043
N	3.0858198	-1.0855906	-0.0197148
N	1.0492552	3.2144714	-0.0277870
S	3.8988957	-4.2394805	0.1191167
S	-0.9707450	5.8321621	0.2361420
S	0.5841472	-5.7313845	0.1239568
S	-4.1545457	4.1553906	0.1233187
S	-4.3514282	-3.9421104	-0.2812538
S	-5.7962545	-0.5293492	-0.0311175
S	5.6756732	0.7603376	-0.1289017
S	3.9531156	4.1025595	-0.0248022
C	1.6401163	-6.5598200	-1.1343737
C	-4.1202724	5.5329102	-1.0949796
C	4.9095335	-3.4434899	-1.2040218
C	0.4994232	6.1982497	-0.8084733
C	-6.7880346	-1.8489234	0.7715624
C	-3.5918987	-5.0690999	0.9628180
C	5.6259071	4.0421999	0.7271755
C	5.9618912	-0.2765792	1.3711268
H	-0.4930854	0.9388800	0.0084858
H	0.3212373	-0.8671758	-0.0270513
H	5.9141159	-3.8716302	-1.0975674
H	0.6647814	7.2761334	-0.6875748
H	1.3545840	-7.6180493	-1.0923246
H	-5.1387934	5.9403678	-1.0844570
H	-4.0720131	-6.0425639	0.8018718
H	-7.8037268	-1.4372137	0.8210476
H	6.9987797	-0.6289422	1.2992304
H	5.9461333	5.0909975	0.7681673
H	4.5065640	-3.6969023	-2.1914550
H	0.2835467	5.9752035	-1.8596000
H	2.7039465	-6.4463542	-0.8988795
H	-3.4013449	6.3100092	-0.8132957
H	4.9390988	-2.3596394	-1.0571621
H	1.3675103	5.6322732	-0.4616204
H	1.4193788	-6.1590696	-2.1303167
H	-3.8915117	5.1444895	-2.0940552
H	-2.5143699	-5.1424902	0.7909055
H	-6.4189040	-2.0364709	1.7864798
H	5.2758620	-1.1296833	1.3721122
H	5.5712572	3.6360644	1.7436117
H	-3.8081157	-4.7171231	1.9784139
H	-6.7821911	-2.7798771	0.1956697
H	5.8416843	0.3239868	2.2804745
H	6.3244302	3.4530056	0.1256600

G (C_s)

N	-1.8950820	0.0236878	0.0000000
N	1.9912895	0.0307254	0.0000000

N	0.0482704	0.0165802	1.9962388
N	0.0482704	0.0165802	-1.9962388
C	-2.7094727	0.1601945	-1.0930391
C	-2.7094727	0.1601945	1.0930391
C	2.8187940	0.0207928	-1.0914308
C	2.8187940	0.0207928	1.0914308
C	-1.0856712	-0.0116029	2.7783874
C	-1.0856712	-0.0116029	-2.7783874
C	1.1834848	-0.0440997	2.7699983
C	1.1834848	-0.0440997	-2.7699983
C	-4.1115709	0.3850951	-0.6916171
C	-4.1115709	0.3850951	0.6916171
C	4.2370844	0.0608345	-0.6907932
C	4.2370844	0.0608345	0.6907932
C	-0.6498048	-0.1463957	4.1605177
C	-0.6498048	-0.1463957	-4.1605177
C	0.7430405	-0.1405029	4.1633205
C	0.7430405	-0.1405029	-4.1633205
N	-2.3449688	0.0796287	-2.3785653
N	-2.3449688	0.0796287	2.3785653
N	2.4438478	-0.0231751	-2.3772953
N	2.4438478	-0.0231751	2.3772953
S	1.9761835	-0.2779847	-5.4064970
S	1.9761835	-0.2779847	5.4064970
S	-1.7806261	-0.3011695	-5.5191505
S	-1.7806261	-0.3011695	5.5191505
S	-5.5232961	0.8083458	-1.6516085
S	-5.5232961	0.8083458	1.6516085
S	5.6826961	-0.0609890	-1.6873075
S	5.6826961	-0.0609890	1.6873075
C	-2.4346264	-1.9992431	-5.2097831
C	-2.4346264	-1.9992431	5.2097831
C	1.1937103	0.3862745	-6.9304265
C	1.1937103	0.3862745	6.9304265
C	-5.3028321	-0.0800063	3.2451252
C	-5.3028321	-0.0800063	-3.2451252
C	5.3196233	1.0399588	3.1201414
C	5.3196233	1.0399588	-3.1201414
H	0.0489027	0.0442593	0.9754042
H	0.0489027	0.0442593	-0.9754042
H	2.0213383	0.4657538	7.6468942
H	2.0213383	0.4657538	-7.6468942
H	-3.1626293	-2.1911880	6.0082313
H	-3.1626293	-2.1911880	-6.0082313
H	0.7794170	1.3831507	6.7409014
H	0.7794170	1.3831507	-6.7409014
H	-2.9361815	-2.0410283	4.2370844
H	-2.9361815	-2.0410283	-4.2370844
H	0.4184595	-0.2794675	7.3169189
H	0.4184595	-0.2794675	-7.3169189
H	-1.6271757	-2.7380553	5.2641221
H	-1.6271757	-2.7380553	-5.2641221

H	6.2066231	0.9695928	3.7621872
H	6.2066231	0.9695928	-3.7621872
H	-6.1971848	0.1757294	3.8272455
H	-6.1971848	0.1757294	-3.8272455
H	5.1966221	2.0747398	2.7795357
H	5.1966221	2.0747398	-2.7795357
H	-5.2752177	-1.1628851	3.0757148
H	-5.2752177	-1.1628851	-3.0757148
H	4.4308933	0.6964787	3.6554184
H	4.4308933	0.6964787	-3.6554184
H	-4.3964807	0.2528803	3.7590815
H	-4.3964807	0.2528803	-3.7590815

H (C_{2v})

N	0.0000000	1.9126345	0.0982361
N	0.0000000	-1.9126345	0.0982361
N	-2.0308116	0.0000000	0.0293123
N	2.0308116	0.0000000	0.0293123
C	-1.0912427	2.7384696	0.1226506
C	-1.0912427	-2.7384696	0.1226506
C	1.0912427	-2.7384696	0.1226506
C	1.0912427	2.7384696	0.1226506
C	-2.7895668	-1.1402583	-0.1481203
C	-2.7895668	1.1402583	-0.1481203
C	2.7895668	1.1402583	-0.1481203
C	2.7895668	-1.1402583	-0.1481203
C	-0.6882008	4.1508144	0.2684534
C	-0.6882008	-4.1508144	0.2684534
C	0.6882008	-4.1508144	0.2684534
C	0.6882008	4.1508144	0.2684534
C	-4.1404676	-0.6999563	-0.4606824
C	-4.1404676	0.6999563	-0.4606824
C	4.1404676	0.6999563	-0.4606824
C	4.1404676	-0.6999563	-0.4606824
N	-2.3772052	2.3921204	-0.0308920
N	-2.3772052	-2.3921204	-0.0308920
N	2.3772052	-2.3921204	-0.0308920
N	2.3772052	2.3921204	-0.0308920
S	-5.5514820	-1.6186263	-0.9627719
S	-5.5514820	1.6186263	-0.9627719
S	5.5514820	1.6186263	-0.9627719
S	5.5514820	-1.6186263	-0.9627719
S	1.7415043	-5.5665447	0.3036493
S	1.7415043	5.5665447	0.3036493
S	-1.7415043	5.5665447	0.3036493
S	-1.7415043	-5.5665447	0.3036493
C	-5.2966648	3.3135290	-0.3112292
C	-5.2966648	-3.3135290	-0.3112292
C	5.2966648	-3.3135290	-0.3112292
C	5.2966648	3.3135290	-0.3112292
C	-2.7889048	-5.1889620	1.7740183

C	-2.7889048	5.1889620	1.7740183
C	2.7889048	5.1889620	1.7740183
C	2.7889048	-5.1889620	1.7740183
H	1.0206614	0.0000000	0.1871864
H	-1.0206614	0.0000000	0.1871864
H	-6.1663668	-3.8746617	-0.6753569
H	-6.1663668	3.8746617	-0.6753569
H	6.1663668	3.8746617	-0.6753569
H	6.1663668	-3.8746617	-0.6753569
H	-4.3672824	-3.7499173	-0.6885198
H	-4.3672824	3.7499173	-0.6885198
H	4.3672824	3.7499173	-0.6885198
H	4.3672824	-3.7499173	-0.6885198
H	-5.2980842	-3.3058096	0.7845177
H	-5.2980842	3.3058096	0.7845177
H	5.2980842	3.3058096	0.7845177
H	5.2980842	-3.3058096	0.7845177
H	-3.5579373	5.9707688	1.8077903
H	-3.5579373	-5.9707688	1.8077903
H	3.5579373	-5.9707688	1.8077903
H	3.5579373	5.9707688	1.8077903
H	-3.2608046	4.2079410	1.6628800
H	-3.2608046	-4.2079410	1.6628800
H	3.2608046	-4.2079410	1.6628800
H	3.2608046	4.2079410	1.6628800
H	-2.1857861	5.2296640	2.6884491
H	-2.1857861	-5.2296640	2.6884491
H	2.1857861	-5.2296640	2.6884491
H	2.1857861	5.2296640	2.6884491

I (C₂)

N	0.0014689	1.9221745	0.0002782
N	-0.0014689	-1.9221745	0.0002782
N	-2.0102783	0.0018646	0.0002287
N	2.0102783	-0.0018646	0.0002287
C	1.0928695	2.7474022	0.0035183
C	-1.0928695	-2.7474022	0.0035183
C	-2.7872666	1.1394286	-0.0022769
C	2.7872666	-1.1394286	-0.0022769
C	1.0882512	-2.7495286	-0.0024177
C	-1.0882512	2.7495286	-0.0024177
C	2.7892500	1.1342958	0.0019848
C	-2.7892500	-1.1342958	0.0019848
C	0.6938298	4.1688916	0.0220339
C	-0.6938298	-4.1688916	0.0220339
C	-4.1782005	0.7013467	-0.0193838
C	4.1782005	-0.7013467	-0.0193838
C	0.6865426	-4.1703157	-0.0195905
C	-0.6865426	4.1703157	-0.0195905
C	4.1794593	0.6938106	0.0174828
C	-4.1794593	-0.6938106	0.0174828

N	2.3826259	2.3918101	0.0091840
N	-2.3826259	-2.3918101	0.0091840
N	-2.3785931	2.3962520	-0.0089098
N	2.3785931	-2.3962520	-0.0089098
S	1.8673207	5.4766061	0.1497076
S	-1.8673207	-5.4766061	0.1497076
S	-5.4992653	1.8651656	-0.1099067
S	5.4992653	-1.8651656	-0.1099067
S	1.8572601	-5.4806158	-0.1461354
S	-1.8572601	5.4806158	-0.1461354
S	5.5025127	1.8555672	0.1063437
S	-5.5025127	-1.8555672	0.1063437
C	1.0939227	-6.5351301	-1.4474520
C	-1.0939227	6.5351301	-1.4474520
C	6.5437194	1.1252703	1.4371053
C	-6.5437194	-1.1252703	1.4371053
C	-1.1057111	-6.5312867	1.4519630
C	1.1057111	6.5312867	1.4519630
C	6.5385527	-1.1369728	-1.4434216
C	-6.5385527	1.1369728	-1.4434216
H	-1.7569279	-7.4097798	1.5377737
H	1.7569279	7.4097798	1.5377737
H	7.4236090	-1.7816267	-1.5076983
H	-7.4236090	1.7816267	-1.5076983
H	-0.0872223	-6.8430772	1.1872452
H	0.0872223	6.8430772	1.1872452
H	6.8400968	-0.1071487	-1.2142789
H	-6.8400968	0.1071487	-1.2142789
H	-1.0886319	-5.9892570	2.4043713
H	1.0886319	5.9892570	2.4043713
H	5.9938324	-1.1620338	-2.3939113
H	-5.9938324	1.1620338	-2.3939113
H	1.7450913	-7.4135684	-1.5342401
H	-1.7450913	7.4135684	-1.5342401
H	7.4269311	1.7722265	1.5036953
H	-7.4269311	-1.7722265	1.5036953
H	0.0757875	-6.8470391	-1.1814901
H	-0.0757875	6.8470391	-1.1814901
H	6.8480894	0.0970731	1.2044897
H	-6.8480894	-0.0970731	1.2044897
H	1.0755751	-5.9929508	-2.3997454
H	-1.0755751	5.9929508	-2.3997454
H	5.9989038	1.1454829	2.3876545
H	-5.9989038	-1.1454829	2.3876545
H	0.9883667	-0.0009860	0.0004060
H	-0.9883667	0.0009860	0.0004060