Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supporting Information

Mechanistic Studies of Photoinduced Intramolecular and Intermolecular Electron Transfer Processes in RuPt-centred Photo-hydrogen-evolving Molecular Devices

Chettiyam Veettil Suneesh, ‡[a] Bijitha Balan,[a] Hironobu Ozawa,[a] Yuki Nakamura,[a]

Tetsuro Katayama,[b] Masayasu Muramatsu,[b] Yutaka Nagasawa,[b]

Hiroshi Miyasaka,*[b] and Ken Sakai*[acd]

[a]*Department of Chemistry, Faculty of Sciences, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581, Japan. E-mail: ksakai@chem.kyushu-univ.jp*

[b]*Division of Frontier Materials Science, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan. E-mail: miyasaka@chem.es.osaka-u.ac.jp*

[c]*International Institute for Carbon Neutral Energy Research (WPI-I2CNER), Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka 819-0395, Japan.*

[d]*Center for Molecular Systems (CMS), Kyushu University, 744 Moto-oka Nishi-ku, Fukuoka 819-0395, Japan.*

‡ Current Address: Department of Chemistry, University of Kerala, Karyavattom Campus, Trivandrum - 695 581, India.

Experimental Details

General Procedures. ^{1}H NMR spectra were measured in CD_3CN and $(CD_3)_2SO$ using a Bruker Avance III (600.13 MHz) spectrometer, where tetramethylsilane (TMS) was used as the internal standard. ESI-TOF (electrospray ionization time-of-flight) mass spectra were acquired on a JEOL JMS-T100CS spectrometer. The elemental analysis was carried out with a Yanaco MT-6 CHN analyzer, at the Service Center of Elemental Analysis of the Faculty of Sciences, Kyushu University. UV-visible absorption spectra were recorded on a Shimadzu UV-2450 spectrophotometer at 20 °C, in air. Emission spectra were acquired on a Shimadzu RF5300PC spectrofluorophotometer.

Emission Decay Measurements. Emission decays in the nanosecond time regime were determined on an Iwatsu DS-4262 digitizing oscilloscope equipped with a Hamamatsu Photonics R928 photomultiplier tube. The excitation source was an N_2 laser (337 nm, Usho KEN-1520). The grating monochromator used was a Jobin Vyvon H-20 instrument. Data acquisitions were carried out up to 512 scans.

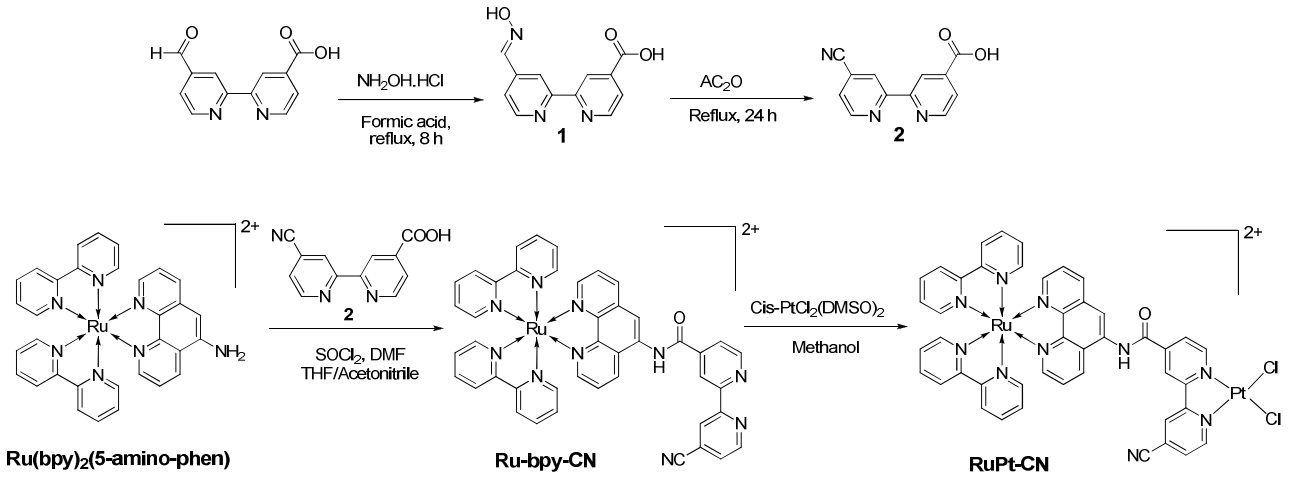
Picosecond Time-correlated Single-photon-counting (TCSPC) Measurements. The light source for the picosecond time-resolved fluorescence (TRF) spectroscopy was the second harmonic (440 nm) of a Ti: sapphire laser (Spectra Physics, Tsunami) generated in a type I BBO crystal (6 mm), and the repetition rate was generally reduced to 320 kHz with a power of 5-10 μW by an EO modulator (Conoptics). The emission was detected at the magic angle configuration utilizing a polarizer and a half-wave-plate. A fused silica sample cell (1.0 cm diameter) was utilized. A photomultiplier-tube (Hamamatsu Photonics, R3809U-50) with an amplifier (Hamamatsu Photonics, C5594) and a counting board (PicoQuanta, PicoHarp 300) were used for the signal detection. A monochromator (Newport,

Oriel 77250) was placed in front of the photomultiplier tube and the observation wavelength was set to 610 nm. The system response time was determined to be 32 ps full-width-at-half-maximum (fwhm) by a scattered light from a colloidal solution. In all the luminescence decay measurements, the sample solutions were purged with Ar for at least 30 min prior to the measurements.

Transient Absorption Spectroscopy. The femtosecond dual NOPA/OPA laser system was used for ultrafast transient absorption spectroscopy. The output of a femtosecond Ti:sapphire laser (Tsunami, Spectra-Physics) pumped by the SHG of a cw Nd_3^+:YVO_4 laser (Millennia Pro, Spectra-Physics) was amplified with 1 kHz repetition rate by using a regenerative amplifier (Spitfire, Spectra-Physics). The amplified pulse (802 nm, 0.9 mJ/pulse energy, 85 fs fwhm, 1 kHz) was divided into two pulses with the same energy (50%). One of the two pulses was guided into an NOPA system (TOPASwhite, Light-Conversion), which covers the wavelength region between 500 and 1000 nm with 1-40 mW output energy with ca. 20-90 fs fwhm. The wavelength of the NOPA was tuned at 880 nm in the present study and was frequency-doubled by a 100 μm BBO crystal. After the compression by a prism pair, the SHG in the UV region (440 nm) was used as a pump pulse with the intensity of 0.3 μJ/pulse. Pulse duration at the sample position was estimated to be ca. 30 fs fwhm by FROG signals. The other pulse at 802 nm was guided into an OPA system (OPA-800, Spectra-Physics) and converted to 1200 nm pulse, which was focused into 2 mm CaF_2 plate to generate a white-light continuum covering the wavelength region from 350 to 1000 nm. This white light was used as a probe pulse. Polarization angle between the pump and probe pulses was set at the magic angle for all of the measurements. The probe pulse was divided into signal and reference pulses and detected with multichannel photodiode array systems (PMA-10, Hamamatsu Photonics) and sent to a personal computer for further analysis. The chirping of the monitoring white-light continuum was corrected for transient absorption spectra. The fwhm of the cross correlation between the pump and probe pulses was ca. 100 fs at the sample position.

Photochemical Hydrogen Evolution Experiments. Hydrogen production from water photocatalyzed by the PHEMDs was followed by using the automated H_2 monitoring system, in which continuous flow of Ar (10 mL/min, controlled by a STEC SEC-E40/PAC-D2 digital mass flow controller) was bubbled through a photolysis solution (10 mL) contained in a Pyrex vial with an inner volume of *ca*. 20 mL. The vent gas from the vial was introduced into a 6-way valve which allowed the automatic injection of the sample gas onto a Shimadzu GC-8A gas chromatograph, equipped with a molecular sieve 5A column (2 m x 3 mm i.d., thermostatted at 30 °C). The injection of the sample gas was controlled by a control software operating on a Windows system and the output signal from the thermal conductivity detector of the gas chromatograph was analyzed in a Shimadzu C-R8A signal integrator which was also controlled within the same control program. Photolysis solutions were deaerated with Ar for at least 30 min prior to the photolysis. The photoirradiation was carried out by an ILC Technology CERMAX LX-300 300 W Xe lamp equipped with a CM-1 cold mirror which reflects lights in the range of $400 < \lambda < 800$ nm. The photolysis vial was immersed in a water bath thermostated at 20 °C to remove IR radiation and to eliminate temperature effects.

Synthesis of 1, 2, Ru-bpy-CN, and RuPt-CN. These were prepared according to the procedures illustrated in Scheme S1. The synthetic details of **1** and **2** are described below, while those of **Ru-bpy-CN** and **RuPt-CN** are reported in the main text.



Scheme S1. Synthetic route to **Ru-bpy-CN** and **RuPt-CN**.

Synthesis of 4'-((hydroxyimino)methyl)l-2,2'-bypyridine-4-carboxylic acid (1). 4'-Formyl-2,2'-bypyridine-4-carboxylic acid (0.5 g, 2.2 mmol) and hydroxylammonium chloride (0.5 g, 7 mmol) were heated at reflux for 6 h in formic acid (95%, 20 mL). After cooled down to room temperature, the reaction mixture was poured into ice cold water (100mL) followed by adjustment of the pH to 2 by adding an aqueous 1 N NaOH solution. The precipitate deposited was collected by filtration, washed with water, and dried in vacuo to afford 4'-((Hydroxyimino)methyl)l-2,2'-bypyridine-4-carboxylic acid (**1)** as a white solid (0.35 g, 66%). ^{1}HNMR (600.13 MHz, [D_6] DMSO, TMS) δ 13.79 (s, 1H), 11.88 (s, 1H), 8.89-8.88 (d, 1H), 8.83 (s, 1H), 8.75-8.74 (d, 1H), 8.61 (s, 1H), 8.32 (s, 1H), 7.90-7.89 (d, 1H), 7.67-7.66 (d, 1H). ESI-TOF MS *m/z* = 266.06 [M+Na^+] (Calcd for $C_{12}H_9N_3NaO_3$: 266.05). Anal. Calcd for $C_{12}H_9N_3O_3$: C 59.26, H 3.73, N 17.28; found: C 59.18, H 3.76, N 17.21.

Synthesis of 4'-Cyano-2,2'-bypyridine-4-carboxylic acid (2). A suspension of **1** (0.3 g, 1.23 mmol), acetic anhydride (15 mL) and sodium acetate (catalytic amount) were heated at reflux for 24 h. After cooled down to room temperature, the reaction mixture was poured into ice cold water (100 mL). The precipitate deposited was collected by filtration, washed with water, and dried in vacuo to afford 4'-cyano-2,2'-bypyridine-4-carboxylic acid (**2**) as a white solid (0.20 g, 73%). ^{1}HNMR (600.13 MHz, [D_6] DMSO, TMS) δ 13.87 (s, 1H), 8.99-8.98 (d, 1H), 8.94-8.93 (d, 1H), 8.82 (s, 1H), 8.69 (s, 1H), 7.99-7.98 (d, 1H), 7.95-7.94 (d, 1H). ESI-TOF MS m/z = 226.06 [M+H$^+$] (Calcd for $C_{12}H_8N_3O_2$: 226.06). Anal. Calcd for $C_{12}H_7N_3O_2 \bullet H_2O$: C 59.26, H 3.73, N 17.28; found: C 59.39, H 3.62, N 17.19.

DFT Calculations. We previously reported in ref. 4c (see references in the main text) only on four selected conformers in their gaseous states (**A-gs**, **B-gs**, **C-gs**, and **D-gs** listed in Table S1), in part due to much slower calculation speed at that time. In this study, eighteen initial structures were generated and were found to fall into 10 energy-minimized structures listed in Table S1. Ten structures were found to be local minima for the gaseous sates (from **A-gs** til **J-gs**). For the water-solvated models (from **A-aq** til **J-aq**), only eight of them were found to be minimum, where the remaining two were found to be transition states (**B-aq** and **C-aq**).

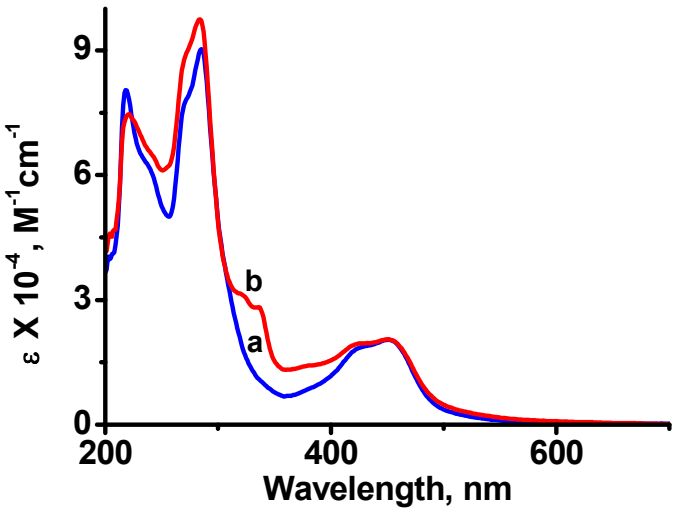


Figure S1. Absorption spectra of [**Ru-bpy-CN**]$(PF_6)_2$•H_2O (a) and [**RuPt-CN**]Cl_2•$7H_2O$ (b) in 0.1 M acetate buffer (pH=5) at 20 ^{0}C in air.

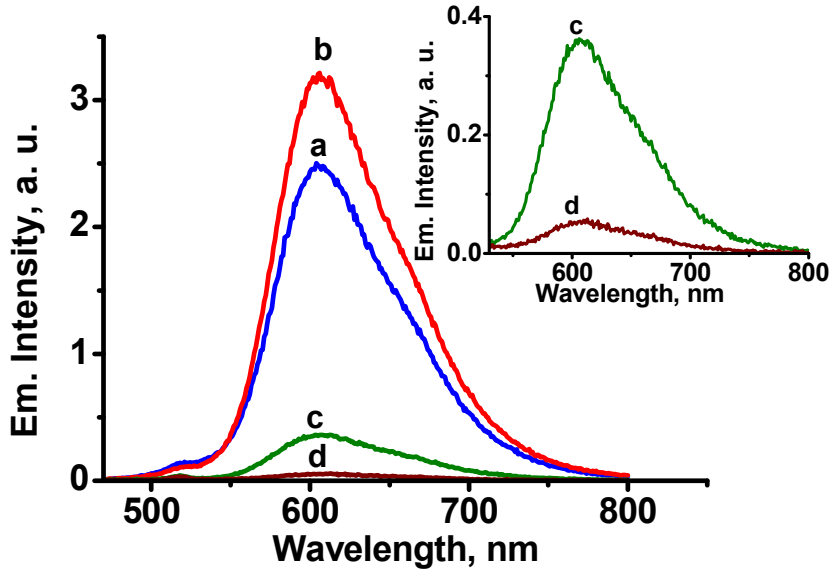


Figure S2. Luminescence spectra of [**Ru-bpy-COOH**]$(PF_6)_2$•H_2O (a), [**Ru-bpy-CN**]$(PF_6)_2$•H_2O (b), [**RuPt-COOH**]Cl_2•$3H_2O$ (c) and [**RuPt-CN**]Cl_2•$7H_2O$ (d) in 0.1 M acetate buffer (pH=5), under Ar at 20 ^{0}C. The excitation wavelength was fixed at 440 nm. All solutions had an equal absorbance at 440 nm (OD=0.1). The inset shows enlarged emission spectra of [**RuPt-COOH**]Cl_2•$3H_2O$ (c) and [**RuPt-CN**]Cl_2•$7H_2O$ (d).

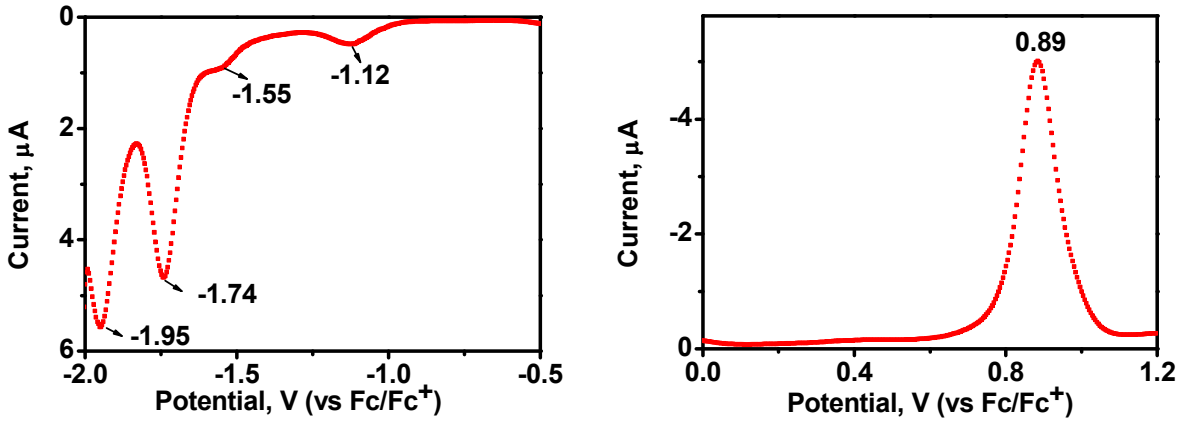


Figure S3. Square wave voltammograms of [**Ru-bpy-CN**]$(PF_6)_2$•H_2O in acetonitrile solution containing 0.1M TBAP (tetra(*n*-butyl)ammonium perchlorate) at room temperature under Ar atmosphere. Each voltammogram was recorded using a glassy carbon disk as the working electrode, at a sweep rate of 50 mVs^{-1}.

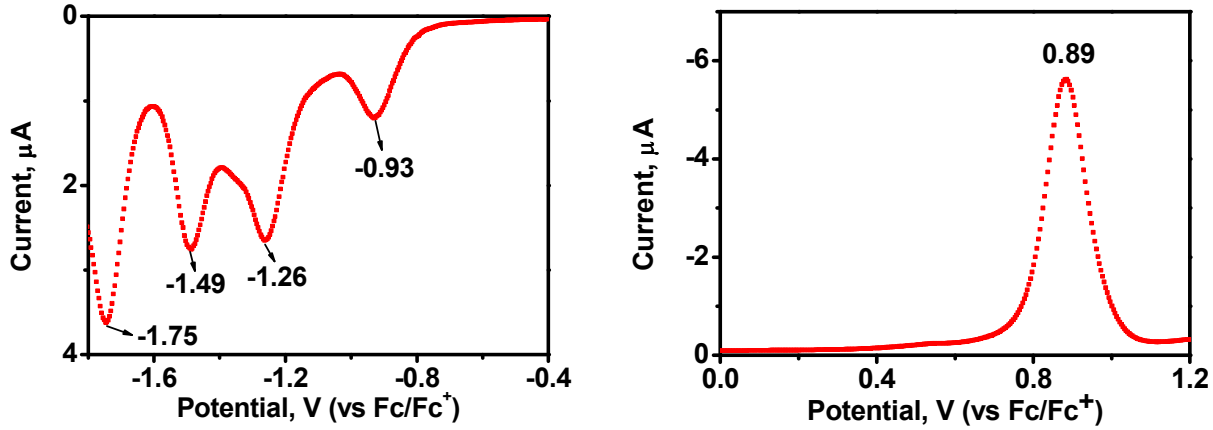


Figure S4. Square wave voltammograms of [**RuPt-CN**]$(PF_6)_2$•$3H_2O$ in acetonitrile solution containing 0.1M TBAP (tetra(*n*-butyl)ammonium perchlorate) at room temperature under Ar atmosphere. Each voltammogram was recorded using a glassy carbon disk as the working electrode, at a sweep rate of 50 mVs^{-1}.

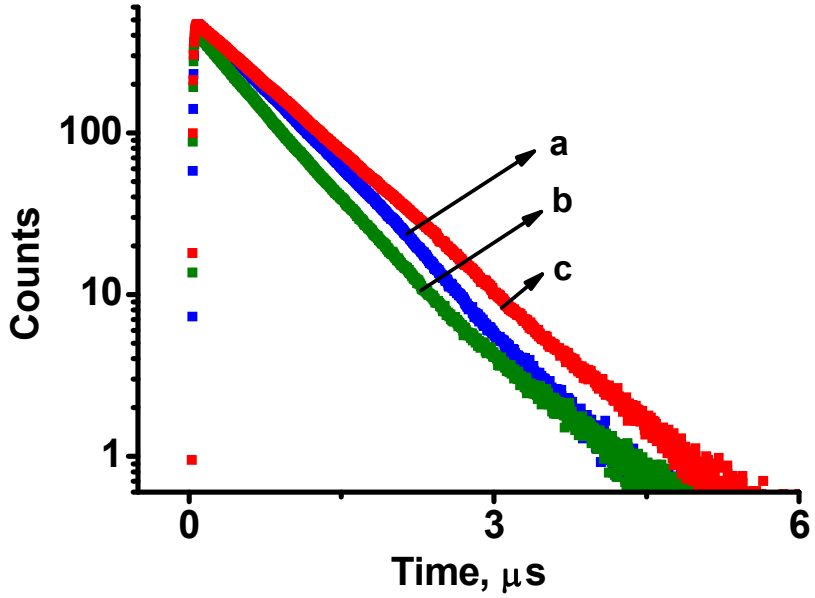


Figure S5. Emission decay profiles at 610 nm for $[Ru(bpy)_2(5\text{-amino-phen})](PF_6)_2 \cdot H_2O$ (a), [**Ru-bpy-COOH**]$(PF_6)_2 \cdot H_2O$ (b) and [**Ru-bpy-CN**]$(PF_6)_2 \cdot H_2O$ (c) in 0.1 M acetate buffer (pH=5) under Ar atmosphere (excitation at 337 nm; N_2 laser).

Table S1. List of 10 conformers computed for **RuPt-COOH**, together with their energy parameters. For all the conformers, gaseous and water-solvated geometries were optimized at the B3LYP level of DFT using the LanL2DZ basis set. Structures in aqueous media were computed using the polarizable continuum model (PCM) method implemented in Gaussian 09.[a]

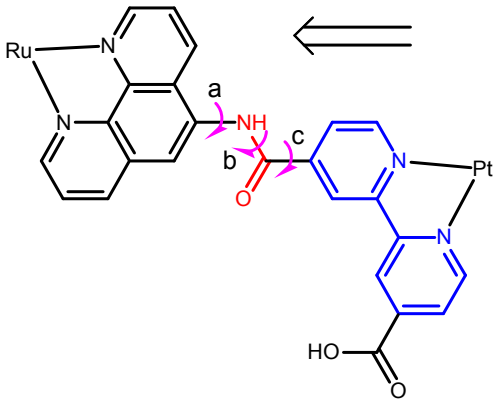
conformer	label	gaseous or solvated state	Total energy not corrected for ZPE (hartree)	Sum of electronic and zero-point energy (hartree)	ZPE (hartree)	ZPCE (kcal/mol)	relative energy (kcal/mol)	LM or TS
A	A-gs	gaseous	-2656.233109	-2655.546539	0.68657	-1666379.353	0.00	LM
	A-aq	water solvated	-2656.472722	-2655.785321	0.68740	-1666529.191	0.00	LM
B	B-gs	gaseous	-2656.232967	-2655.546416	0.68655	-1666379.276	0.08	LM
	B-aq	water solvated	-2656.473025	-2655.785969	0.68706	-1666529.598	-0.41	TS
C	C-gs	gaseous	-2656.225642	-2655.539302	0.68634	-1666374.812	4.54	LM
	C-aq	water solvated	-2656.472412	-2655.7853	0.68711	-1666529.178	0.01	TS
D	D-gs	gaseous	-2656.22566	-2655.539367	0.68629	-1666374.853	4.50	LM
	D-aq	water solvated	-2656.472363	-2655.785053	0.68731	-1666529.023	0.17	LM
E	E-gs	gaseous	-2656.230278	-2655.54405	0.68623	-1666377.791	1.56	LM
	E-aq	water solvated	-2656.470848	-2655.784071	0.68678	-1666528.407	0.78	LM
F	F-gs	gaseous	-2656.230278	-2655.54405	0.68623	-1666377.791	1.56	LM
	F-aq	water solvated	-2656.471209	-2655.784249	0.68696	-1666528.518	0.67	LM
G	G-gs	gaseous	-2656.226662	-2655.540513	0.68615	-1666375.572	3.78	LM
	G-aq	water solvated	-2656.469421	-2655.782513	0.68691	-1666527.429	1.76	LM
H	H-gs	gaseous	-2656.226663	-2655.540513	0.68615	-1666375.572	3.78	LM
	H-aq	water solvated	-2656.470646	-2655.783597	0.68705	-1666528.109	1.08	LM
I	I-gs	gaseous	-2656.230663	-2655.544477	0.68619	-1666378.059	1.29	LM
	I-aq	water solvated	-2656.471209	-2655.784249	0.68696	-1666528.518	0.67	LM
J	J-gs	gaseous	-2656.227065	-2655.540985	0.68608	-1666375.868	3.49	LM
	J-aq	water solvated	-2656.470617	-2655.783951	0.68667	-1666528.331	0.86	LM

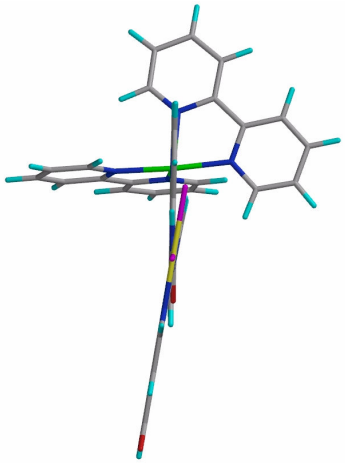
[a]Abbreviations are definded as follows: ZPE = zero point energy; ZPCE = energy corrected for zero-point energy; LM = local minimum; TS = transition state. LM denotes that the final structure was confirmed to be placed at a stationary point and was characterized as a minimum by their harmonic vibrational frequencies. Eighteen strucutures out of these twenty cases were confirmed to be located at the LM, but two solvated strucures (B-aq and C-aq) gave TM's instead of their LM characters in gaseous state. This was repeatedly checked to be correct.

Table S2. Structural features of each formers defined by dihedral angles of the carbamoyl (NCO) and bipyridyl plane (bpy) with respect to the phenanthroline plane (phen).[a]

conformer	dihedral angle (esd) (dgree)	
	phen-NCO	phen-bpy
A-aq	-1.540(1)	-9.139(1)
B-aq	10.278(1)	36.721(2)
C-aq	5.823(1)	-142.294(1)
D-aq	-9.631(1)	137.818(1)
E-aq	112.680(1)	134.549(1)
F-aq	118.683(1)	95.919(1)
G-aq	124.916(1)	-12.745(1)
H-aq	114.704(1)	-97.169(1)
I-aq	-108.612(1)	-74.887(1)
J-aq	-114.659(1)	97.196(1)

[a]This table shows dihedral angles between the three planes determined by the best plane calculations. For each DFT-optimized structure, twelve N/C atoms of phen, three N/C/O atoms of the bridging carbamoyl CONH group, and 10 N/C atoms of bpy were used to define the least-squares planes. Therefore the values in parentheses correspond to the estimated standard deviations given in the least-squares calculations. Definition of angles in this table is explained as follows. As shown by the figure in the left side, two types of dihedral cants can be defined. One is the cant of NCO with regard to phen due to the rotations around the N-C(phen) and N-C(CO) bonds, while the other is that of bpy with regard to phen. The figure in the left below shows a case in which the cant of NCO with regard to phen is zero, and the counter clockwise rotation of the C=O group is supposed to have a positive value for the dihedral cant. In the same manner, the position shown below in the left corresponds to a case in which bpy has a cant of zero degree with regard to phen. The definition of a positive value of the cant is defined in the same way. For instance, the figure in the right below corresponds to the structure of A-aq, which has a negative value of cant for bpy/phen.





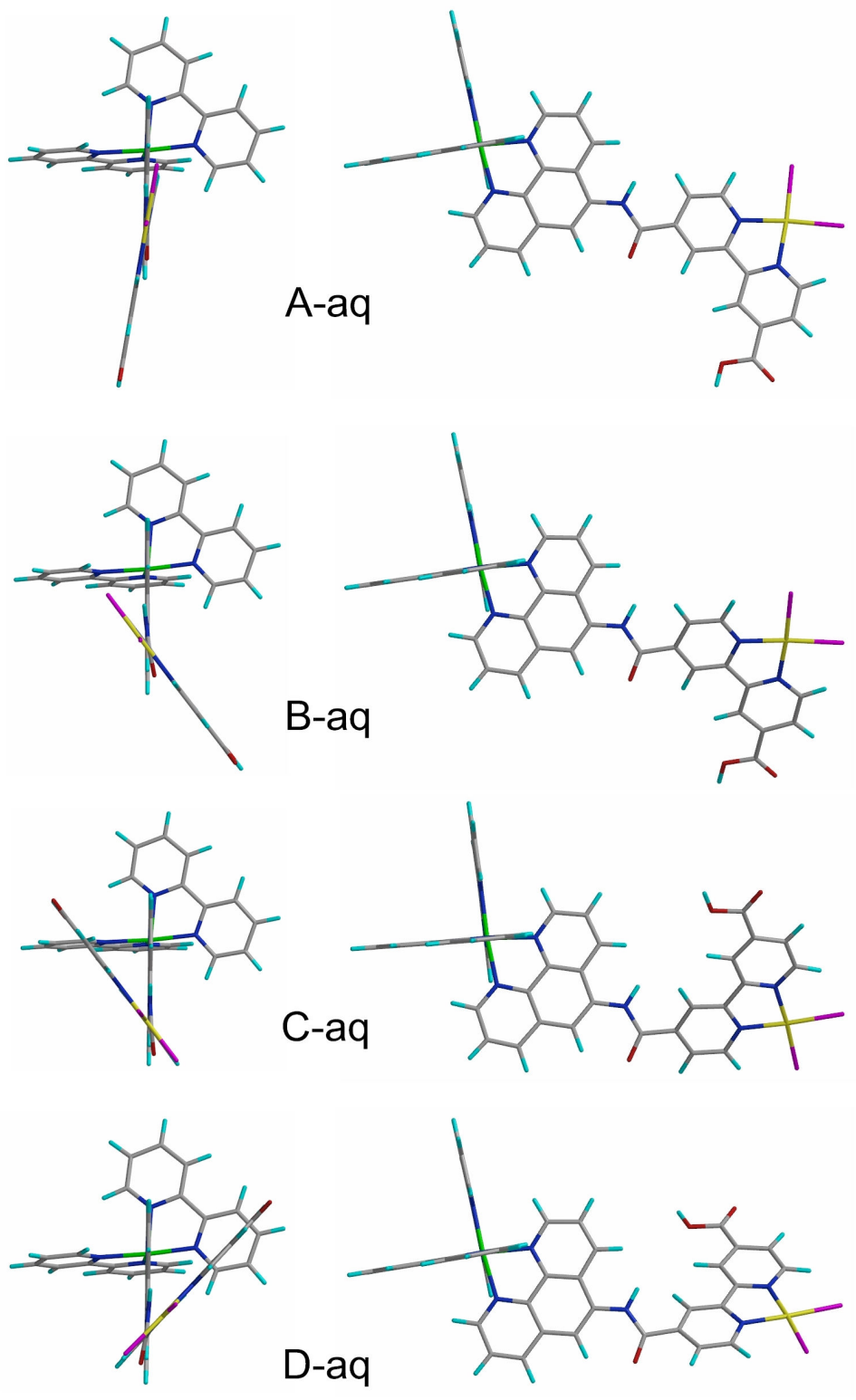


Figure S6. Structures of all the ten structures optimized by DFT using polarizable continuum model (PCM) for modeling the structures in water, where those optimized for the gaseous state are omitted although the coordinates are all supplied as tables (*vide infra*). Views in two directions are shown for each structure.

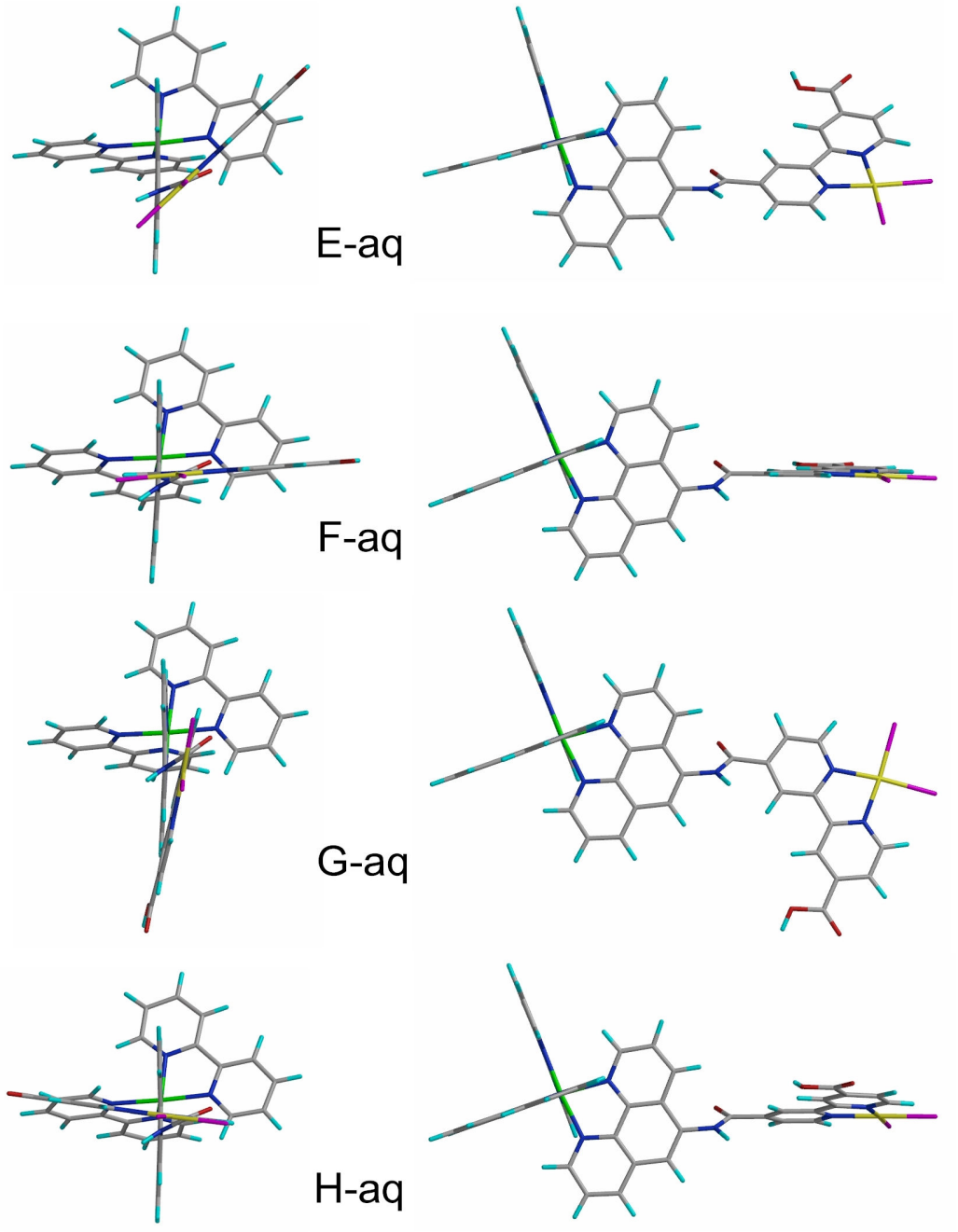


Figure S6 (continued).

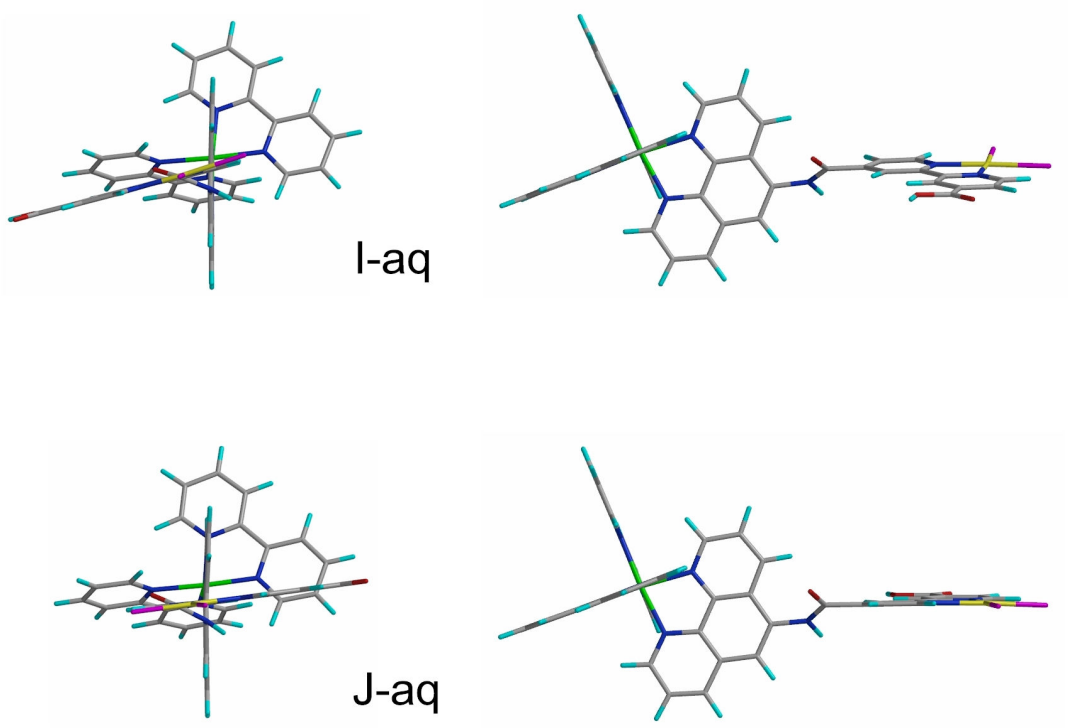


Figure S6 (continued).

Picosecond luminescence studies

Table S3. Picosecond emission lifetime data for [**RuPt-COOH**]Cl_2•$3H_2O$ under Ar atmosphere under various experimental c onditions.[a]

SI No	Experiment condition	Lifetime (% composition)		
		T_1	T_2	T_3
1	pH = 5	285 ps (74.4%)	3.87 ns (17 %)	285 ns (9%)
2	pH =5+0.1 M NaCl	285 ps (70%)	3.89 ns (19%)	424 ns (10.6%)
3	pH =3+0.1 M NaCl	277 ps (64.5)	3.94 ns (25.6%)	120 ns (9.8%)
4	pH =4+0.1 M NaCl	280 ps (69.9%)	3.75 ns (19.9%)	246 ns (10.1%)
5	pH =6+0.1 M NaCl	286 ps (68.3%)	3.44 ns (20.5%)	472 ns (11.1%)

[a] All the pH conditions, other than pH 3 were adjusted using 0.1 M acetate buffer (Using different ratios of sodium acetate and acetic acid). pH 3 was adjusted using dilute sulphuric acid. The reliability of the estimated values of T3 is not very high due to the fact that the decay profiles in these experiments were obtained using the picosecond setup.

Table S4. Picosecond emission lifetime data for [**RuPt-CN**]Cl_2•$7H_2O$ under Ar atmosphere under various experimental conditions.[a]

SI No	Experiment condition	Lifetime (% composition)		
		T_1	T_2	T_3
1	pH = 5	49.7 ps (76.7%)	452 ps (14.2%)	3.53 ns (7.9%)
2	pH =5+0.1 M NaCl	53.7 ps (76.7%)	425 ps (14.1%)	3.55 ns (8%)
3	pH =3+0.1 M NaCl	63.9 ps (77.5%)	476 ps (11.8%)	3.69 ns (9.6%)
4	pH =6+0.1 M NaCl	62.2 ps (75.1%)	575 ps (15%)	3.68 ns (8.6%)

[a] All the pH conditions, other than pH 3 were adjusted using 0.1 M acetate buffer (Using different ratios of sodium acetate and acetic acid). pH 3 was adjusted using dilute sulphuric acid.

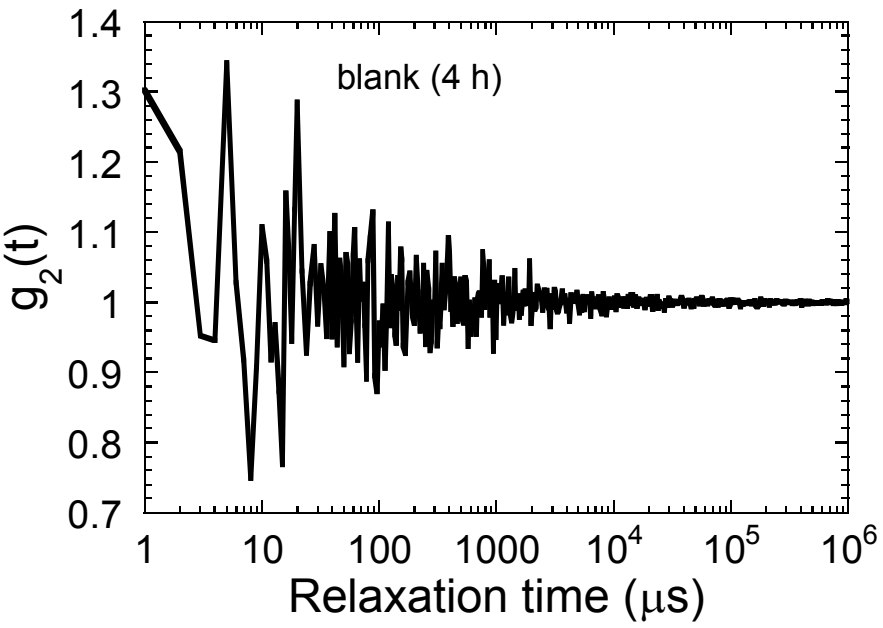


Figure S7. Autocorrelation function obtained by the dynamic light scattering (DLS) apparatus for an aqueous acetate buffer solution (0.03 M CH_3CO_2H and 0.07 M CH_3CO_2Na; pH 5.0, 10mL) containing 30 mM EDTA after 4 h of irradiation with 300 W Xe lamp (this is a control experiment) under Ar atmosphere, revealing the lack of any features ascribable to either metal or metal oxide dispersion.

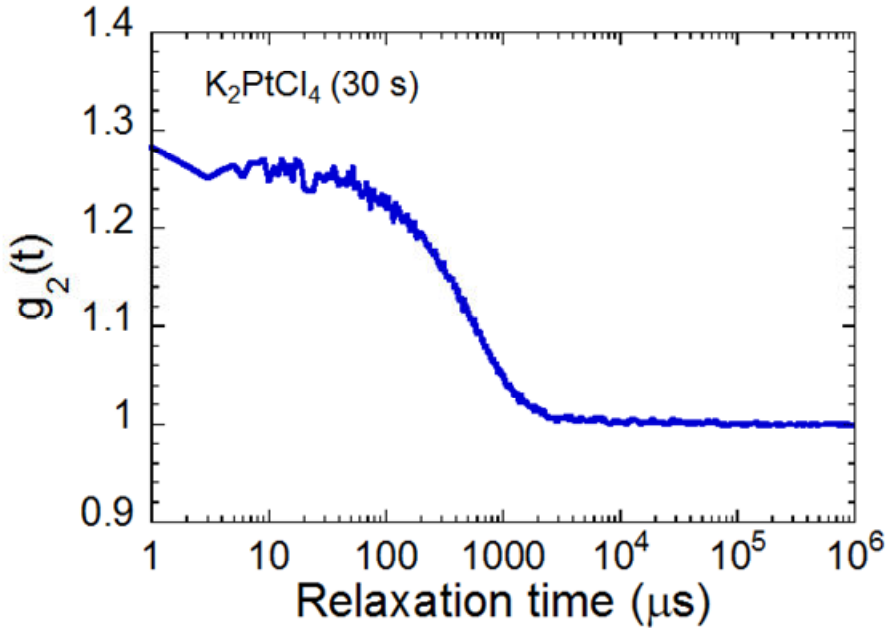


Figure S8. Autocorrelation function obtained by the DLS measurement for an aqueous acetate buffer solution (0.03 M CH_3CO_2H and 0.07 M CH_3CO_2Na; pH 5.0, 10mL) containing 30 mM EDTA, 0.04 mM $[Ru(bpy)_3]Cl_2 \cdot 6H_2O$, 2 mM $[MV]Cl_2$ (MV^{2+} = N,N'-dimethyl-4,4'-bipyridinium), and 0.1 mM K_2PtCl_4 after 30 s of irradiation with 300 W Xe lamp under Ar atmosphere.

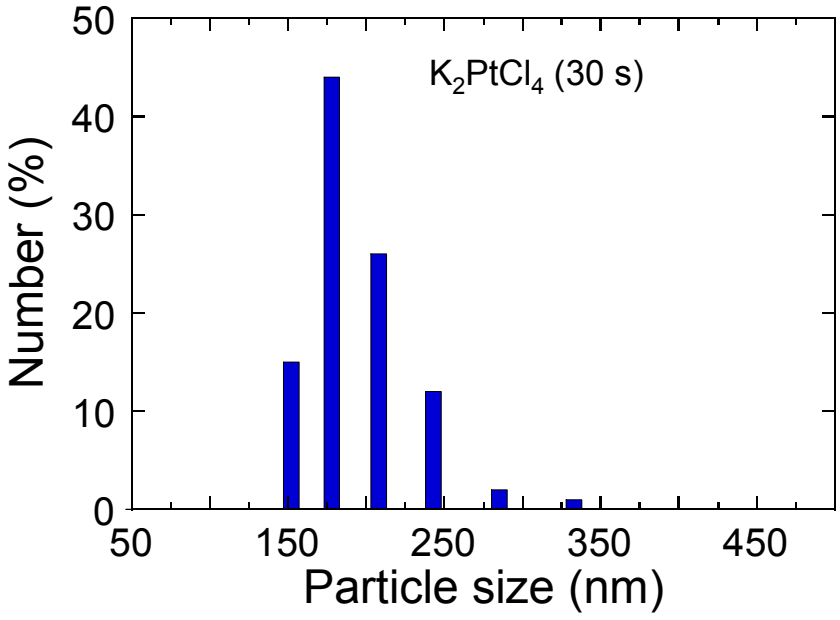


Figure S9. Particle size distribution determined from the DLS data depicted in Figure S6, showing the presence of colloidal platinum particles having diameters in the range 150-350 nm.

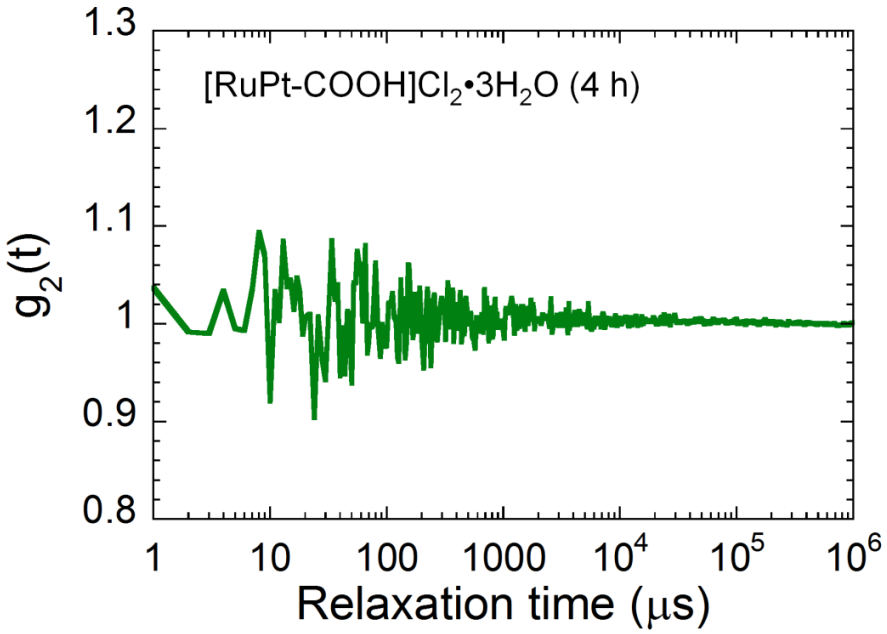


Figure S10. Autocorrelation function obtained by the DLS measurement for an aqueous acetate buffer solution (0.03M CH_3CO_2H and 0.07 M CH_3CO_2Na; pH 5.0, 10mL) containing both 30 mM EDTA and 0.1 mM [**RuPt-COOH**]Cl_2•$3H_2O$ after 4 h of irradiation with 300 W Xe lamp under Ar atmosphere, revealing the lack of any decay feature ascribable to colloidal metal dispersion.

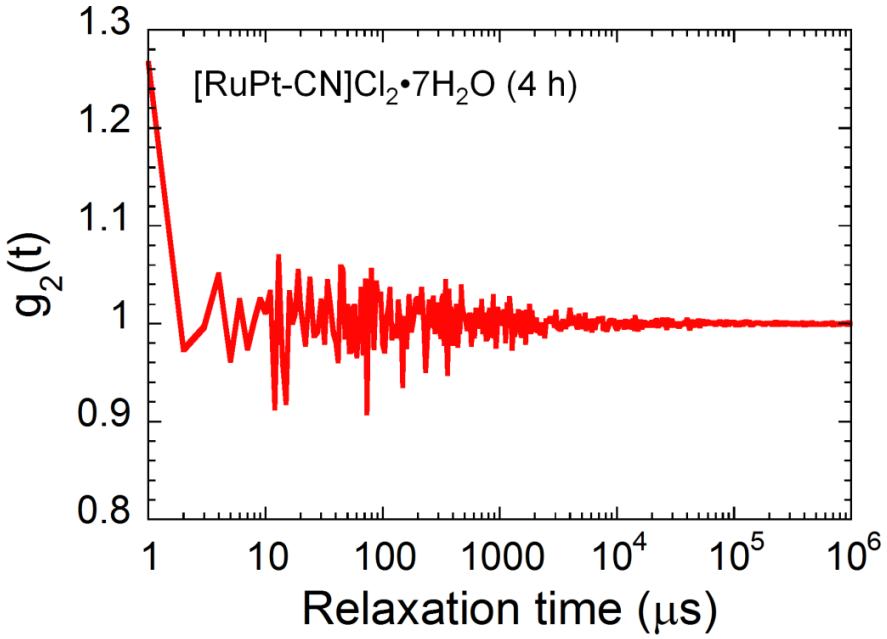


Figure S11. Autocorrelation function obtained by the DLS measurement for an aqueous acetate buffer solution (0.03M CH_3CO_2H and 0.07 M CH_3CO_2Na; pH 5.0, 10mL) containing both 30 mM EDTA and 0.1 mM [**RuPt-CN**]$Cl_2 \cdot 7H_2O$ after 4 h of irradiation with 300 W Xe lamp under Ar atmosphere, revealing the lack of any decay feature ascribable to colloidal metal dispersion.

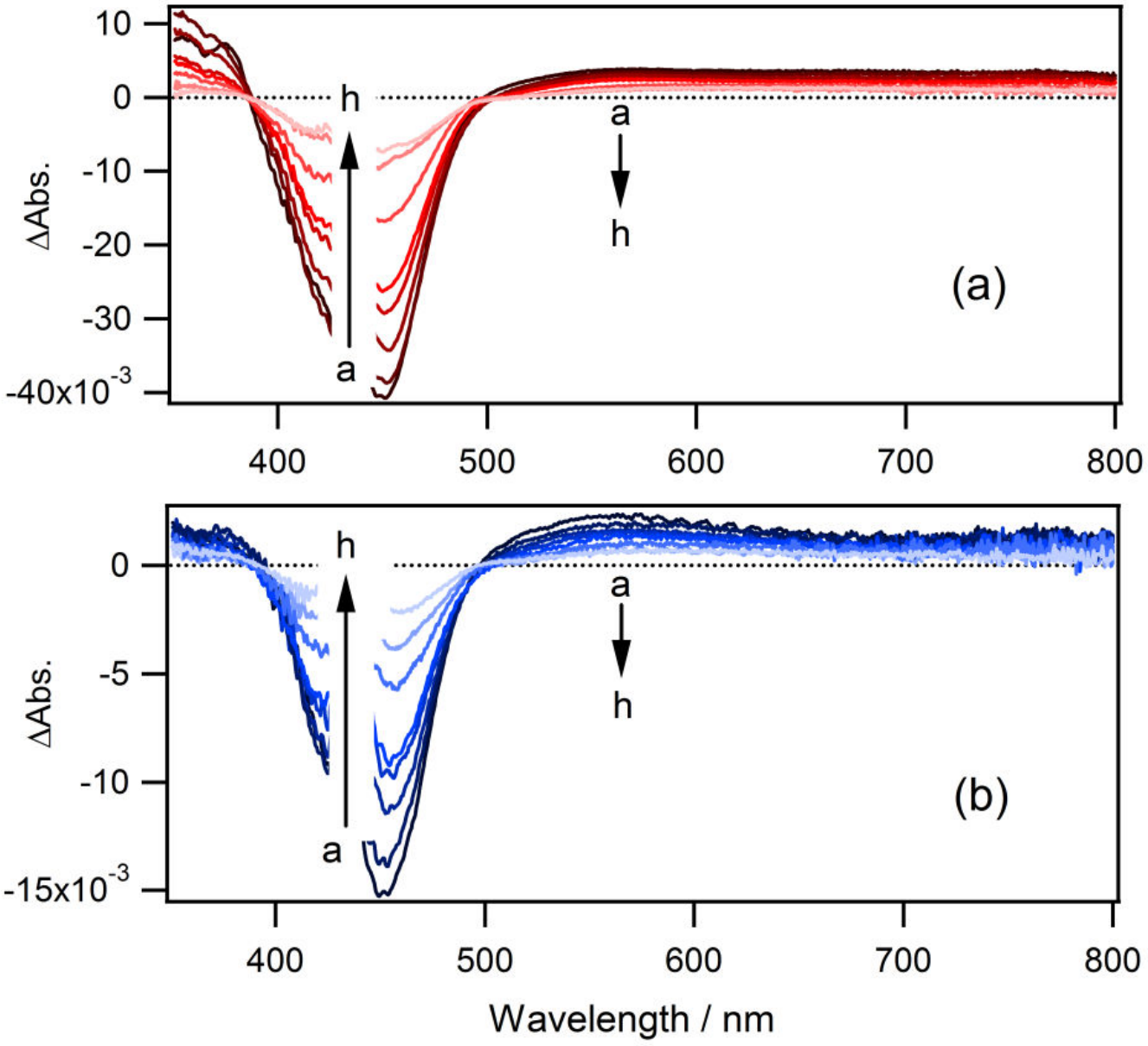


Figure S12. Femtosecond transient absorption spectra obtained for [**RuPt-CN**]Cl_2•$7H_2O$ (a) and [**RuPt-COOH**]Cl_2•$3H_2O$ (b) in 0.1 M acetate buffer solution (pH=5) under Ar atmosphere. The spectral data were recorded after 0.1, 0.5, 1, 5, 10, 100, 500 and 2000 ps (a-h) following laser pulse excitation (440 nm).

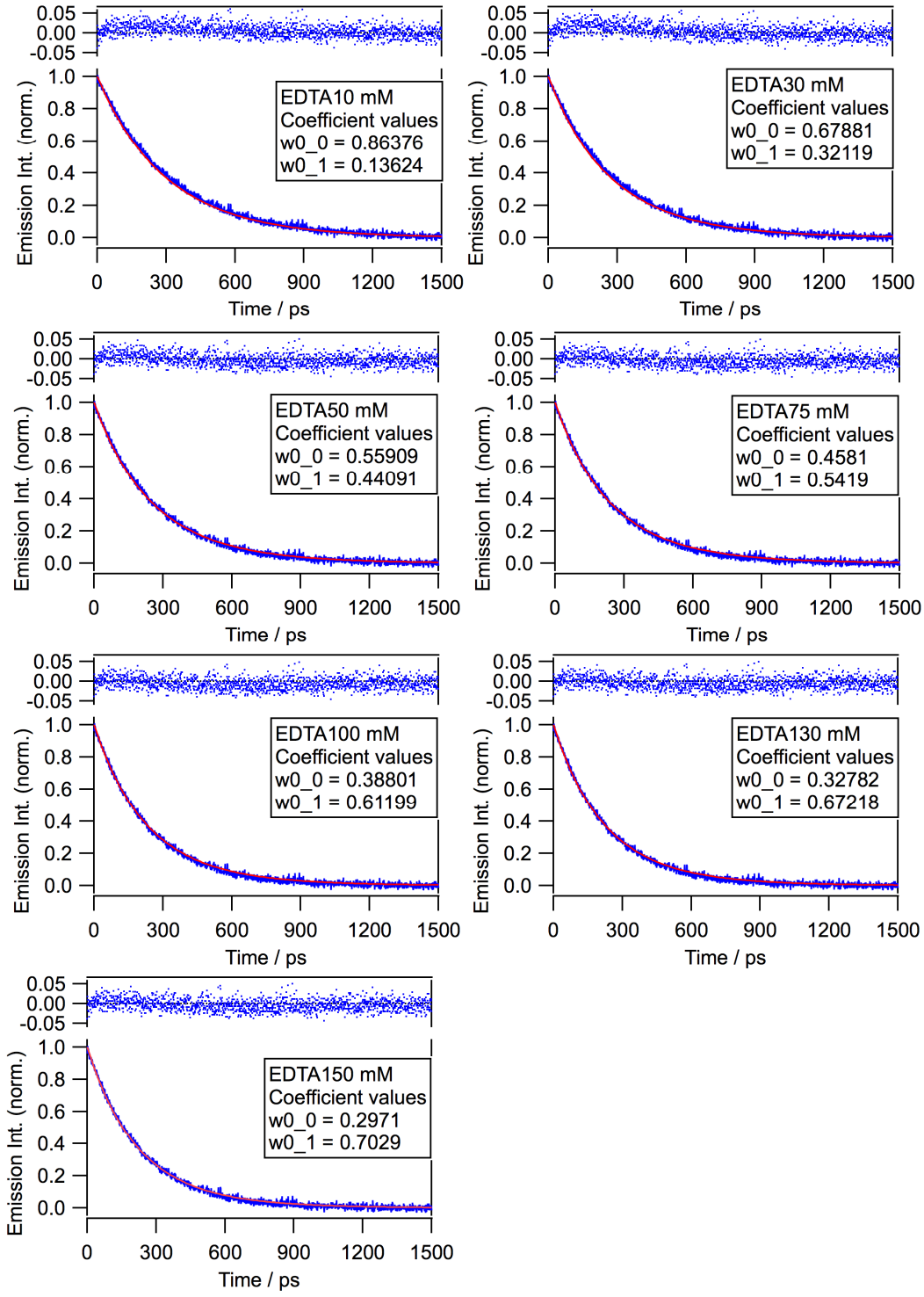


Figure S13. The shortest lifetime components of the emission decay profiles at 610 nm for [**RuPt-COOH**]Cl_2•$3H_2O$ in 0.1 M acetate buffer (pH=5) under Ar atmosphere (excitation at 440 nm; Ti:Sapphire laser) at various EDTA concentrations. The shortest lifetime component for each data was once extracted based on the least-squares fitting analysis and was then combined with the noise data for each run. Finally, each data set was fitted to eq. 3 to determine the scaling factors w0_0 and w0_1 together with the τ' value. The τ' values determined are plotted in Figure 8.

Table S5. Cartesian coordinates for **A-gs**.

Pt1	-7.820889	-1.495544	0.229350
Cl2	-10.091822	-2.123723	0.557561
Cl3	-7.139157	-3.786014	0.405754
N4	-8.213146	0.495908	0.060727
C5	-8.509898	3.264622	-0.202115
C6	-9.452677	1.055408	0.123531
C7	-7.102174	1.294366	-0.131855
C8	-7.231541	2.683787	-0.265961
C9	-9.632887	2.437609	-0.004401
N10	-5.940448	-0.805525	-0.048048
C11	-3.408325	0.361009	-0.384021
C12	-5.824914	0.565728	-0.184556
C13	-4.828585	-1.590816	-0.104509
C14	-3.557486	-1.041574	-0.272859
C15	-4.566042	1.160153	-0.354108
C16	-2.091253	1.049965	-0.565702
N17	-0.961175	0.301428	-0.192691
O18	-2.008000	2.220554	-1.007326
C19	0.391525	0.662550	-0.334107
C20	3.174883	1.266489	-0.637886
C21	0.793251	1.846996	-0.938861
C22	1.398798	-0.271437	0.178560
C23	2.777643	0.052486	0.011214
C24	2.180979	2.168249	-1.101966
C25	1.106300	-1.493329	0.849082
N26	3.800093	-0.765555	0.462402
C27	2.144074	-2.310357	1.297598
C28	3.484076	-1.920163	1.085805
N29	4.529697	1.503133	-0.776915
C30	2.626425	3.369732	-1.728151
C31	3.994141	3.602923	-1.858447
C32	4.923055	2.649445	-1.372068
C33	-8.714993	4.737241	-0.338966
O34	-9.814640	5.302494	-0.291929
O35	-7.522435	5.416181	-0.527082
Ru36	5.728848	-0.027676	0.031064
N37	6.770640	-1.712573	0.725185
C38	8.187247	-4.037874	1.432585
C39	7.294876	-1.856003	1.974285
C40	6.945650	-2.724139	-0.195405
C41	7.651708	-3.894048	0.143120
C42	8.004642	-2.998902	2.364825
N43	7.565109	0.917415	-0.330306
C44	10.030836	2.244256	-0.593464
C45	8.002535	1.768179	0.662128
C46	8.341407	0.730900	-1.433620
C47	9.573751	1.375267	-1.602393
C48	9.234902	2.438609	0.546271
N49	5.948618	1.140867	1.761691
C50	6.412417	2.828810	3.964014
C51	7.092749	1.908122	1.817876
C52	5.050622	1.215752	2.783133
C53	5.246651	2.042315	3.897017
C54	7.339743	2.757747	2.912830
N55	5.737886	-1.250724	-1.675794
C56	5.804896	-3.069445	-3.820212
C57	6.352726	-2.475426	-1.525960
C58	5.167077	-0.937252	-2.872314
C59	5.181875	-1.815091	-3.963975
C60	6.393400	-3.397625	-2.588849
H61	-10.273503	0.363935	0.277445
H62	-6.369195	3.320303	-0.420510

H63	-10.626951	2.868543	0.047223
H64	-5.010380	-2.657074	-0.013283
H65	-2.723986	-1.732817	-0.359558
H66	-4.462687	2.233329	-0.466359
H67	-1.159037	-0.589174	0.241887
H68	0.041978	2.540805	-1.293883
H69	0.087521	-1.816375	1.037348
H70	1.936434	-3.243039	1.810560
H71	4.304974	-2.538399	1.427753
H72	1.900743	4.088546	-2.096975
H73	4.365801	4.506864	-2.328855
H74	5.989407	2.813917	-1.468667
H75	-7.673564	6.384457	-0.619755
H76	7.788901	-4.684450	-0.585534
H77	8.403108	-3.067746	3.371349
H78	8.734156	-4.935594	1.702656
H79	7.955838	0.055232	-2.186413
H80	10.156688	1.196522	-2.499503
H81	9.575623	3.102905	1.331724
H82	10.982551	2.756574	-0.691924
H83	4.166572	0.596766	2.695725
H84	4.503350	2.067573	4.686604
H85	8.239258	3.361059	2.949686
H86	6.593194	3.481354	4.812206
H87	7.134410	-1.035982	2.662654
H88	4.698774	0.036330	-2.944010
H89	4.716081	-1.520509	-4.898244
H90	6.874293	-4.360671	-2.463795
H91	5.831452	-3.773356	-4.645907

Table S6. Cartesian coordinates for **A-aq**.

Pt1	-7.887342	-1.467625	0.258841
Cl2	-10.243863	-2.053647	0.470662
Cl3	-7.300334	-3.816374	0.556762
N4	-8.217137	0.519475	-0.006421
C5	-8.427945	3.281939	-0.380052
C6	-9.441775	1.111579	-0.033663
C7	-7.078470	1.281951	-0.164650
C8	-7.164533	2.667940	-0.352400
C9	-9.580190	2.490825	-0.219209
N10	-5.968456	-0.834214	0.058348
C11	-3.401700	0.272931	-0.227480
C12	-5.819462	0.524276	-0.126691
C13	-4.870751	-1.633145	0.091045
C14	-3.578812	-1.113891	-0.051065
C15	-4.547582	1.088301	-0.268639
C16	-2.070720	0.966703	-0.403588
N17	-0.943600	0.217257	-0.136955
O18	-2.038489	2.174177	-0.768921
C19	0.412149	0.617739	-0.240722
C20	3.174047	1.317984	-0.408984
C21	0.786623	1.901341	-0.602210
C22	1.429899	-0.392163	0.056908
C23	2.799160	-0.012341	-0.028786
C24	2.169738	2.275959	-0.695708
C25	1.160315	-1.739830	0.428595
N26	3.837404	-0.885196	0.242814
C27	2.215883	-2.611678	0.691721
C28	3.547391	-2.155388	0.591327
N29	4.523162	1.602498	-0.482799
C30	2.592162	3.583668	-1.068074

C31	3.956111	3.863074	-1.133798
C32	4.899231	2.850499	-0.834687
C33	-8.581317	4.755068	-0.576487
O34	-9.674911	5.346972	-0.611787
O35	-7.373485	5.392853	-0.715218
Ru36	5.745961	-0.030590	0.012844
N37	6.822924	-1.789834	0.366974
C38	8.301121	-4.166401	0.609720
C39	7.315471	-2.179449	1.574517
C40	7.057414	-2.574939	-0.740759
C41	7.796524	-3.767543	-0.637497
C42	8.054533	-3.358225	1.735268
N43	7.553272	1.015840	-0.104273
C44	9.970894	2.443918	-0.032431
C45	7.948345	1.649113	1.053826
C46	8.346587	1.090971	-1.207721
C47	9.557362	1.794827	-1.210700
C48	9.156319	2.368073	1.107624
N49	5.904195	0.742565	1.953495
C50	6.291026	1.915136	4.476538
C51	7.021867	1.510775	2.194911
C52	4.993898	0.561305	2.948995
C53	5.152935	1.128003	4.219823
C54	7.231224	2.106060	3.452313
N55	5.823090	-0.864660	-1.908009
C56	5.995037	-2.184389	-4.381064
C57	6.482948	-2.070084	-2.003687
C58	5.255313	-0.326119	-3.021441
C59	5.322146	-0.953062	-4.272041
C60	6.578352	-2.745047	-3.234406
H61	-10.293456	0.457429	0.095538
H62	-6.274079	3.269645	-0.477012
H63	-10.566725	2.938622	-0.237170
H64	-5.050855	-2.690819	0.229224
H65	-2.759681	-1.823216	-0.034344
H66	-4.418942	2.153231	-0.415429
H67	-1.101422	-0.728771	0.182034
H68	0.028739	2.640756	-0.820063
H69	0.151308	-2.126718	0.515534
H70	2.029314	-3.641055	0.974545
H71	4.380176	-2.815073	0.797160
H72	1.855111	4.347026	-1.296616
H73	4.315536	4.847008	-1.412998
H74	5.961796	3.050277	-0.886408
H75	-7.468407	6.364637	-0.843821
H76	7.979535	-4.378181	-1.513047
H77	8.425022	-3.627571	2.717971
H78	8.872577	-5.084175	0.700246
H79	7.994262	0.582517	-2.095251
H80	10.154680	1.828060	-2.114844
H81	9.461896	2.861561	2.021956
H82	10.904272	2.996143	-0.001777
H83	4.134125	-0.052554	2.715760
H84	4.401474	0.953324	4.981539
H85	8.111163	2.710534	3.634860
H86	6.443395	2.369062	5.450106
H87	7.105307	-1.533592	2.416624
H88	4.748468	0.621649	-2.897865
H89	4.856284	-0.484081	-5.131401
H90	7.095982	-3.693952	-3.302562
H91	6.063385	-2.696382	-5.335150

Table S7. Cartesian coordinates for **B-gs**.

Pt1	7.822483	-1.511272	-0.176794
Cl2	10.090176	-2.198900	0.035153
Cl3	7.150440	-3.776490	-0.574106
N4	8.206427	0.462116	0.151019
C5	8.491336	3.211771	0.576177
C6	9.441688	0.991434	0.368930
C7	7.093942	1.281348	0.141308
C8	7.217435	2.661903	0.351774
C9	9.615780	2.363416	0.584952
N10	5.943338	-0.776978	-0.312868
C11	3.409184	0.430449	-0.384500
C12	5.821828	0.585261	-0.108006
C13	4.837215	-1.525581	-0.581875
C14	3.565156	-0.954858	-0.625832
C15	4.561838	1.200211	-0.142503
C16	2.089872	1.138447	-0.400568
N17	0.961691	0.317143	-0.227855
O18	2.003548	2.381497	-0.540747
C19	-0.391688	0.701338	-0.263442
C20	-3.175231	1.373601	-0.337861
C21	-0.795548	1.999854	-0.547427
C22	-1.397079	-0.331326	0.006431
C23	-2.776207	0.028838	-0.045911
C24	-2.183092	2.357538	-0.590849
C25	-1.102861	-1.688201	0.323936
N26	-3.797128	-0.879222	0.180940
C27	-2.139195	-2.592484	0.556632
C28	-3.479619	-2.157228	0.475671
N29	-4.529546	1.649996	-0.352038
C30	-2.629921	3.680925	-0.878868
C31	-3.997261	3.948869	-0.897513
C32	-4.924273	2.911084	-0.629451
C33	8.690297	4.673731	0.805374
O34	9.785902	5.212321	1.006725
O35	7.497076	5.376124	0.768423
Ru36	-5.726952	-0.033155	0.054658
N37	-6.766456	-1.759586	0.641998
C38	-8.178083	-3.978110	1.641624
C39	-7.300741	-2.684046	-0.204059
C40	-6.927502	-1.922842	2.001540
C41	-7.631592	-3.027260	2.517706
C42	-8.008129	-3.802628	0.255120
N43	-7.561440	0.928779	-0.267645
C44	-10.019143	2.136313	-0.910390
C45	-8.009650	0.935518	-1.571372
C46	-8.324471	1.511719	0.698517
C47	-9.552477	2.124477	0.417745
C48	-9.237475	1.535428	-1.909371
N49	-5.974251	-0.280325	-2.015900
C50	-6.469934	-0.439081	-4.780341
C51	-7.117154	0.277558	-2.547762
C52	-5.094073	-0.905026	-2.846555
C53	-5.306264	-1.006653	-4.227447
C54	-7.379660	0.207316	-3.929087
N55	-5.710191	0.155341	2.145999
C56	-5.745878	0.180250	4.957966
C57	-6.321214	-0.867495	2.839483
C58	-5.128289	1.172625	2.840270
C59	-5.127123	1.221587	4.240323
C60	-6.346461	-0.870547	4.247055
H61	10.264054	0.284780	0.363597
H62	6.353896	3.315278	0.342255

H63	10.606304	2.770750	0.756659
H64	5.024192	-2.580217	-0.757990
H65	2.736812	-1.604090	-0.894855
H66	4.453674	2.267479	0.013211
H67	1.162538	-0.652049	-0.023899
H68	-0.045502	2.758163	-0.732040
H69	-0.083548	-2.052722	0.400453
H70	-1.930009	-3.628114	0.801270
H71	-4.300338	-2.842794	0.646762
H72	-1.905509	4.464626	-1.079833
H73	-4.369997	4.944158	-1.114310
H74	-5.990210	3.103846	-0.635042
H75	7.644310	6.338232	0.915577
H76	-7.758344	-3.148383	3.587143
H77	-8.414994	-4.512288	-0.457249
H78	-8.723339	-4.832513	2.029726
H79	-7.932169	1.483351	1.707166
H80	-10.124768	2.576636	1.220624
H81	-9.585609	1.535892	-2.935615
H82	-10.967482	2.600850	-1.160944
H83	-4.211409	-1.327892	-2.383922
H84	-4.576709	-1.514764	-4.848858
H85	-8.278149	0.650861	-4.341870
H86	-6.662860	-0.497803	-5.846763
H87	-7.150073	-2.514429	-1.262735
H88	-4.664323	1.954440	2.252364
H89	-4.652485	2.053312	4.749795
H90	-6.825043	-1.678955	4.787261
H91	-5.760225	0.186954	6.043198

Table S8. Cartesian coordinates for **B-aq**.

Pt1	7.855005	-1.480467	-0.006859
Cl2	10.197864	-2.093966	0.280148
Cl3	7.310395	-3.847589	-0.204206
N4	8.156226	0.521118	0.158707
C5	8.335326	3.302684	0.361004
C6	9.361655	1.111100	0.381179
C7	7.021108	1.294472	0.031900
C8	7.091682	2.690455	0.131633
C9	9.484123	2.500206	0.486536
N10	5.946194	-0.832359	-0.249914
C11	3.395330	0.287260	-0.575355
C12	5.783356	0.536980	-0.203892
C13	4.870446	-1.634188	-0.459238
C14	3.584234	-1.107499	-0.625194
C15	4.517900	1.110070	-0.372835
C16	2.063056	0.962899	-0.782970
N17	0.953694	0.223501	-0.424006
O18	2.013517	2.135747	-1.244168
C19	-0.411012	0.583109	-0.553580
C20	-3.188470	1.188530	-0.793684
C21	-0.821203	1.717852	-1.232930
C22	-1.396394	-0.310448	0.056388
C23	-2.775189	0.011695	-0.087103
C24	-2.213714	2.043604	-1.366447
C25	-1.084703	-1.488517	0.792621
N26	-3.785997	-0.772718	0.438074
C27	-2.112830	-2.267648	1.321140
C28	-3.457144	-1.885591	1.125521
N29	-4.544180	1.437318	-0.875901
C30	-2.674999	3.199536	-2.058214

C31	-4.045811	3.438381	-2.141829
C32	-4.957310	2.537622	-1.539809
C33	8.470831	4.786119	0.476343
O34	9.547849	5.378345	0.668187
O35	7.266669	5.432743	0.347692
Ru36	-5.716812	-0.022561	0.075089
N37	-6.723727	-1.462461	1.211266
C38	-8.075169	-3.246012	2.909648
C39	-7.258706	-2.614697	0.722222
C40	-6.855925	-1.175032	2.552409
C41	-7.528716	-2.057359	3.417233
C42	-7.937626	-3.528653	1.537843
N43	-7.562895	0.765602	-0.512809
C44	-10.045020	1.667892	-1.468225
C45	-8.034472	0.329494	-1.731812
C46	-8.312186	1.635221	0.218346
C47	-9.553608	2.108255	-0.225266
C48	-9.275695	0.770987	-2.225037
N49	-5.989606	-0.944967	-1.786508
C50	-6.531653	-2.032486	-4.319257
C51	-7.150215	-0.610408	-2.448839
C52	-5.112165	-1.803505	-2.374390
C53	-5.348364	-2.367126	-3.634480
C54	-7.437791	-1.145528	-3.717870
N55	-5.672498	0.845811	1.982340
C56	-5.662581	1.792176	4.626785
C57	-6.253608	0.101431	2.985225
C58	-5.097935	2.041068	2.288366
C59	-5.074884	2.546674	3.594202
C60	-6.256628	0.559448	4.315461
H61	10.210733	0.446836	0.470397
H62	6.204543	3.302165	0.035708
H63	10.455371	2.946836	0.663465
H64	5.065037	-2.697703	-0.495964
H65	2.774449	-1.800843	-0.822110
H66	4.383310	2.184280	-0.354652
H67	1.141077	-0.669759	0.013272
H68	-0.086030	2.378149	-1.671678
H69	-0.063219	-1.806378	0.969907
H70	-1.895401	-3.167034	1.885325
H71	-4.268417	-2.481781	1.522233
H72	-1.961773	3.881102	-2.511042
H73	-4.434306	4.307299	-2.660725
H74	-6.024482	2.711873	-1.589457
H75	7.349920	6.410962	0.424186
H76	-7.628968	-1.824667	4.470223
H77	-8.345452	-4.433962	1.102474
H78	-8.595723	-3.933314	3.568197
H79	-7.899352	1.952762	1.166473
H80	-10.113917	2.801355	0.392008
H81	-9.642002	0.423503	-3.183265
H82	-11.003634	2.014276	-1.840020
H83	-4.215124	-2.039345	-1.817453
H84	-4.620233	-3.047777	-4.061008
H85	-8.351848	-0.876913	-4.232932
H86	-6.743777	-2.451364	-5.297315
H87	-7.131669	-2.799111	-0.336213
H88	-4.660632	2.593358	1.467358
H89	-4.606606	3.504925	3.788882
H90	-6.712541	-0.032562	5.099459
H91	-5.659112	2.154643	5.649372

Table S9. Cartesian coordinates for **C-gs**.

Pt1	-8.112171	-0.645286	0.294429
Cl2	-10.267652	0.127800	0.944854
Cl3	-8.836993	-2.908919	0.515581
N4	-7.328882	1.216931	0.066878
C5	-6.045438	3.672912	-0.318078
C6	-8.021047	2.379929	0.227677
C7	-5.992893	1.249047	-0.283995
C8	-5.336082	2.471130	-0.484237
C9	-7.406923	3.623118	0.043988
N10	-6.223046	-1.141303	-0.248713
C11	-3.532296	-1.607598	-0.890219
C12	-5.366055	-0.074796	-0.433876
C13	-5.771747	-2.417675	-0.422241
C14	-4.442335	-2.679186	-0.755588
C15	-4.012160	-0.291852	-0.742034
C16	-2.111564	-1.948000	-1.222456
N17	-1.136014	-1.067150	-0.715824
O18	-1.816366	-2.974391	-1.875021
C19	0.262018	-1.178598	-0.862094
C20	3.115030	-1.364627	-1.059164
C21	0.852536	-2.130601	-1.683979
C22	1.105857	-0.251839	-0.102050
C23	2.523463	-0.365517	-0.220102
C24	2.277283	-2.239536	-1.799180
C25	0.617344	0.766195	0.765564
N26	3.401602	0.462468	0.459311
C27	1.511118	1.595032	1.443895
C28	2.900886	1.417883	1.270380
N29	4.495350	-1.429423	-1.102283
C30	2.911054	-3.210548	-2.629462
C31	4.302851	-3.260719	-2.676167
C32	5.068949	-2.356758	-1.898666
C33	-5.402653	5.001115	-0.521426
O34	-5.971961	6.092829	-0.403222
O35	-4.057664	4.895980	-0.866600
Ru36	5.434286	0.000675	0.123081
N37	6.204502	1.363657	1.522548
C38	7.260474	3.008253	3.546164
C39	6.624793	2.629097	1.243164
C40	6.306878	0.893287	2.814772
C41	6.832489	1.703951	3.838800
C42	7.154202	3.478478	2.223382
N43	7.395384	-0.485896	-0.436178
C44	10.019760	-0.958779	-1.332158
C45	7.873797	0.164833	-1.553463
C46	8.210258	-1.355684	0.223544
C47	9.521611	-1.619033	-0.192976
C48	9.184835	-0.060054	-2.014272
N49	5.695436	1.201615	-1.578014
C50	6.231968	2.669840	-3.916805
C51	6.920336	1.089340	-2.200674
C52	4.754145	2.028247	-2.112746
C53	4.984102	2.777242	-3.273916
C54	7.204225	1.816814	-3.372031
N55	5.396421	-1.138992	1.886163
C56	5.375016	-2.466693	4.365508
C57	5.839464	-0.493451	3.020701
C58	4.950295	-2.422334	1.984693
C59	4.926078	-3.117642	3.200671
C60	5.834246	-1.143625	4.269356
H61	-9.064197	2.269069	0.503151
H62	-4.294650	2.512067	-0.777599

H63	-7.973188	4.539012	0.174132
H64	-6.512270	-3.197124	-0.275833
H65	-4.110256	-3.700229	-0.905363
H66	-3.367668	0.565719	-0.909933
H67	-1.486671	-0.339124	-0.107642
H68	0.224456	-2.819056	-2.233961
H69	-0.444656	0.921431	0.926619
H70	1.153932	2.373395	2.109278
H71	3.612460	2.049478	1.787850
H72	2.308073	-3.899609	-3.213373
H73	4.816379	-3.985840	-3.298253
H74	6.151556	-2.389052	-1.917028
H75	-3.675923	5.790224	-1.020852
H76	6.913481	1.327709	4.851865
H77	7.475803	4.478532	1.953036
H78	7.668565	3.640387	4.328361
H79	7.793265	-1.844736	1.094900
H80	10.132640	-2.321251	0.363910
H81	9.556389	0.457324	-2.890935
H82	11.032194	-1.138921	-1.679207
H83	3.806697	2.082193	-1.591353
H84	4.203904	3.423003	-3.662313
H85	8.167332	1.721440	-3.859566
H86	6.441185	3.234341	-4.819859
H87	6.528895	2.955074	0.215029
H88	4.614818	-2.888965	1.067130
H89	4.563927	-4.139718	3.229424
H90	6.181313	-0.630776	5.158687
H91	5.367603	-2.976657	5.323550

Table S10. Cartesian coordinates for **C-aq**.

Pt1	-8.130144	-0.540635	0.248062
Cl2	-10.359073	0.370244	0.625961
Cl3	-9.043888	-2.788827	0.514692
N4	-7.230308	1.262456	0.006535
C5	-5.791653	3.626978	-0.383768
C6	-7.861215	2.464979	0.088014
C7	-5.878341	1.208604	-0.263354
C8	-5.141818	2.383800	-0.463205
C9	-7.169433	3.665348	-0.102030
N10	-6.225462	-1.159217	-0.101716
C11	-3.536196	-1.778985	-0.596744
C12	-5.315098	-0.148809	-0.316984
C13	-5.820544	-2.457382	-0.145181
C14	-4.488772	-2.796767	-0.396646
C15	-3.965605	-0.440079	-0.565979
C16	-2.114800	-2.188983	-0.888679
N17	-1.136817	-1.328837	-0.428554
O18	-1.880846	-3.266303	-1.500293
C19	0.266950	-1.437753	-0.592006
C20	3.105641	-1.559860	-0.856382
C21	0.855420	-2.445048	-1.338218
C22	1.094329	-0.424905	0.064814
C23	2.506843	-0.507907	-0.088473
C24	2.281960	-2.526673	-1.485664
C25	0.595659	0.649743	0.854141
N26	3.376729	0.403398	0.481789
C27	1.483626	1.558586	1.427910
C28	2.872019	1.410354	1.223580
N29	4.483958	-1.580555	-0.940784
C30	2.923911	-3.549171	-2.240670

C31	4.315130	-3.556640	-2.327412
C32	5.069136	-2.557716	-1.665568
C33	-5.058168	4.911665	-0.592341
O34	-5.584231	6.037081	-0.528784
O35	-3.726779	4.715666	-0.864992
Ru36	5.405734	-0.006054	0.100107
N37	6.160083	1.520919	1.317287
C38	7.204836	3.410515	3.114121
C39	6.490293	2.771457	0.893534
C40	6.343901	1.188317	2.641648
C41	6.866698	2.121855	3.554871
C42	7.011708	3.740754	1.759762
N43	7.357882	-0.459057	-0.496563
C44	9.960190	-0.902788	-1.456734
C45	7.761761	0.105780	-1.686455
C46	8.233041	-1.230341	0.204613
C47	9.537288	-1.475508	-0.242689
C48	9.061348	-0.105713	-2.181973
N49	5.538938	1.038314	-1.711338
C50	5.916005	2.316278	-4.184097
C51	6.742731	0.925126	-2.371894
C52	4.538961	1.772082	-2.271811
C53	4.689875	2.424801	-3.501832
C54	6.948864	1.558787	-3.610889
N55	5.498633	-0.964309	1.961011
C56	5.642055	-2.033702	4.554209
C57	5.956765	-0.189626	3.003982
C58	5.119703	-2.249000	2.202615
C59	5.178216	-2.817582	3.481223
C60	6.034279	-0.708818	4.309228
H61	-8.920655	2.436107	0.304150
H62	-4.082251	2.350066	-0.679289
H63	-7.695283	4.610267	-0.033453
H64	-6.584856	-3.203568	0.025660
H65	-4.196900	-3.839308	-0.435501
H66	-3.277294	0.372905	-0.763486
H67	-1.462345	-0.551965	0.132479
H68	0.237021	-3.192220	-1.816038
H69	-0.464086	0.793881	1.032529
H70	1.122956	2.382822	2.032018
H71	3.576407	2.109514	1.654723
H72	2.330741	-4.310051	-2.738213
H73	4.838802	-4.318610	-2.893423
H74	6.150381	-2.554513	-1.717036
H75	-3.239108	5.559470	-1.005478
H76	7.011255	1.853319	4.594094
H77	7.258297	4.724253	1.375845
H78	7.608733	4.137944	3.810386
H79	7.872018	-1.655673	1.131566
H80	10.197804	-2.098246	0.350060
H81	9.371952	0.342361	-3.117718
H82	10.964671	-1.072440	-1.829976
H83	3.612389	1.835466	-1.716687
H84	3.865035	2.999687	-3.907469
H85	7.897500	1.466180	-4.125358
H86	6.064998	2.809327	-5.138987
H87	6.326175	2.989107	-0.153377
H88	4.773316	-2.820905	1.352082
H89	4.866410	-3.846047	3.624200
H90	6.392183	-0.093288	5.125263
H91	5.697411	-2.443704	5.557142

Table S11. Cartesian coordinates for **D-gs**.

Pt1	8.095033	-0.723965	0.363398
Cl2	10.247245	0.007247	1.071079
Cl3	8.770886	-3.001724	0.596126
N4	7.351625	1.153066	0.123097
C5	6.121728	3.632850	-0.284234
C6	8.063381	2.302699	0.293674
C7	6.022193	1.210607	-0.248914
C8	5.391898	2.444745	-0.460216
C9	7.476142	3.557262	0.099114
N10	6.209571	-1.183568	-0.223700
C11	3.524065	-1.599079	-0.914664
C12	5.374045	-0.101076	-0.413617
C13	5.741163	-2.450586	-0.419118
C14	4.414082	-2.687094	-0.780155
C15	4.021137	-0.292850	-0.742516
C16	2.103563	-1.904334	-1.279606
N17	1.135528	-1.044155	-0.723974
O18	1.800738	-2.882937	-1.997930
C19	-0.261294	-1.118832	-0.902382
C20	-3.109148	-1.201411	-1.203819
C21	-0.845160	-1.928014	-1.868574
C22	-1.109437	-0.313557	-0.019622
C23	-2.524695	-0.373625	-0.191188
C24	-2.267701	-1.983750	-2.037724
C25	-0.627384	0.522667	1.027389
N26	-3.407343	0.338059	0.604259
C27	-1.525412	1.242031	1.816210
C28	-2.912560	1.131389	1.577662
N29	-4.487262	-1.201894	-1.313579
C30	-2.895303	-2.800104	-3.024305
C31	-4.284934	-2.794270	-3.127811
C32	-5.054990	-1.984617	-2.256067
C33	5.507897	4.972869	-0.500426
O34	6.095631	6.053751	-0.372411
O35	4.168488	4.891796	-0.870709
Ru36	-5.435049	0.032091	0.104075
N37	-6.214614	1.429242	1.463458
C38	-7.287527	3.449591	3.101047
C39	-6.646207	1.147639	2.724571
C40	-6.312873	2.722213	0.994379
C41	-6.847218	3.744595	1.801334
C42	-7.184198	2.126293	3.570429
N43	-7.393673	-0.513658	-0.410545
C44	-10.015375	-1.395050	-0.924927
C45	-7.886078	-1.632410	0.227051
C46	-8.193871	0.154838	-1.287344
C47	-9.503242	-0.254101	-1.571281
C48	-9.195954	-2.085965	-0.018789
N49	-5.723646	-1.672919	1.296431
C50	-6.294699	-4.015363	2.746024
C51	-6.949558	-2.288979	1.162253
C52	-4.798771	-2.215379	2.136590
C53	-5.046013	-3.378677	2.876872
C54	-7.250562	-3.462047	1.879949
N55	-5.373617	1.797853	-1.026677
C56	-5.343675	4.277841	-2.352709
C57	-5.829211	2.930498	-0.386342
C58	-4.908115	1.899004	-2.302943
C59	-4.879407	3.115337	-2.997297
C60	-5.820222	4.179439	-1.036024
H61	9.099804	2.172256	0.585416
H62	4.356205	2.505169	-0.770198

H63	8.057976	4.462251	0.236757
H64	6.466302	-3.243293	-0.267042
H65	4.069794	-3.700991	-0.949989
H66	3.390371	0.575062	-0.909042
H67	1.490159	-0.363348	-0.065085
H68	-0.215670	-2.543924	-2.497239
H69	0.431634	0.611249	1.247771
H70	-1.173886	1.881787	2.618289
H71	-3.627215	1.676777	2.181682
H72	-2.289565	-3.416700	-3.681768
H73	-4.793877	-3.403975	-3.866558
H74	-6.136020	-1.969191	-2.323939
H75	3.804465	5.792045	-1.032397
H76	-6.925176	4.758262	1.426014
H77	-7.514290	1.854256	4.567251
H78	-7.702322	4.230392	3.730532
H79	-7.766755	1.027330	-1.765476
H80	-10.102134	0.309799	-2.278343
H81	-9.578472	-2.963827	0.488415
H82	-11.026695	-1.736639	-1.121065
H83	-3.850032	-1.699008	2.209868
H84	-4.278104	-3.772980	3.533701
H85	-8.214381	-3.944437	1.767307
H86	-6.517090	-4.919973	3.302946
H87	-6.552316	0.119177	3.050004
H88	-4.561554	0.982770	-2.764175
H89	-4.503614	3.145969	-4.014392
H90	-6.178816	5.066838	-0.527755
H91	-5.335223	5.235783	-2.862876

Table S12. Cartesian coordinates for **D-aq**.

Pt1	8.128788	-0.612655	0.257573
Cl2	10.371075	0.262500	0.642390
Cl3	9.016183	-2.877471	0.472063
N4	7.243594	1.205834	0.089706
C5	5.812126	3.595291	-0.142556
C6	7.885006	2.398977	0.215333
C7	5.886210	1.173634	-0.154816
C8	5.152574	2.361563	-0.272980
C9	7.197209	3.611405	0.103895
N10	6.216817	-1.201511	-0.102717
C11	3.526709	-1.778908	-0.639083
C12	5.313370	-0.175804	-0.269916
C13	5.803713	-2.493596	-0.209305
C14	4.471160	-2.811805	-0.483716
C15	3.963163	-0.445702	-0.538338
C16	2.106017	-2.158720	-0.971064
N17	1.130427	-1.330140	-0.451742
O18	1.870699	-3.182477	-1.667985
C19	-0.270784	-1.402570	-0.652268
C20	-3.099770	-1.428869	-1.017138
C21	-0.851747	-2.298842	-1.533477
C22	-1.102227	-0.471803	0.111829
C23	-2.510913	-0.510486	-0.087322
C24	-2.273189	-2.327363	-1.737504
C25	-0.611576	0.476257	1.053840
N26	-3.386357	0.317279	0.591982
C27	-1.503685	1.311856	1.724238
C28	-2.888493	1.210250	1.471925
N29	-4.471510	-1.387054	-1.169550
C30	-2.906152	-3.221022	-2.647519

C31	-4.291630	-3.172704	-2.792710
C32	-5.048501	-2.243676	-2.038712
C33	5.080937	4.893114	-0.256808
O34	5.615937	6.010652	-0.146052
O35	3.740624	4.719213	-0.499079
Ru36	-5.404557	0.030457	0.068990
N37	-6.158585	1.585879	1.247044
C38	-7.173119	3.803614	2.640599
C39	-6.632560	1.449377	2.515451
C40	-6.184244	2.826348	0.648174
C41	-6.688483	3.947821	1.331446
C42	-7.144244	2.531658	3.242403
N43	-7.362202	-0.487626	-0.450675
C44	-10.000164	-1.307244	-0.958104
C45	-7.924279	-1.504993	0.288708
C46	-8.098581	0.112350	-1.425447
C47	-9.415819	-0.269815	-1.708371
C48	-9.244263	-1.927996	0.048234
N49	-5.798740	-1.517276	1.426359
C50	-6.516559	-3.651093	3.106626
C51	-7.046783	-2.091408	1.320973
C52	-4.922414	-1.996369	2.351187
C53	-5.244727	-3.057052	3.207212
C54	-7.422613	-3.161212	2.153628
N55	-5.236325	1.660045	-1.236620
C56	-5.052819	3.983923	-2.803148
C57	-5.654916	2.870688	-0.729398
C58	-4.734036	1.605532	-2.500300
C59	-4.628220	2.742120	-3.311792
C60	-5.570279	4.044540	-1.500148
H61	8.948803	2.352893	0.405616
H62	4.087280	2.344457	-0.460661
H63	7.730873	4.548617	0.208501
H64	6.562757	-3.251980	-0.071891
H65	4.173642	-3.849366	-0.576461
H66	3.279359	0.378936	-0.700856
H67	1.456803	-0.608425	0.178522
H68	-0.230803	-2.992399	-2.083401
H69	0.444378	0.572852	1.281120
H70	-1.149494	2.040062	2.444424
H71	-3.595830	1.845175	1.989321
H72	-2.310090	-3.925612	-3.218905
H73	-4.808395	-3.835753	-3.477188
H74	-6.124342	-2.189953	-2.144749
H75	3.254280	5.572034	-0.575608
H76	-6.706485	4.919759	0.853898
H77	-7.508537	2.374161	4.251304
H78	-7.563689	4.662173	3.176692
H79	-7.614527	0.902785	-1.983494
H80	-9.962376	0.237070	-2.495638
H81	-9.680279	-2.727211	0.634789
H82	-11.019262	-1.625396	-1.151300
H83	-3.955240	-1.513951	2.401607
H84	-4.513601	-3.403216	3.929063
H85	-8.404252	-3.609804	2.062982
H86	-6.796333	-4.475888	3.753568
H87	-6.592418	0.456968	2.944333
H88	-4.422600	0.632769	-2.857198
H89	-4.223708	2.649065	-4.313359
H90	-5.900985	4.992929	-1.094803
H91	-4.983623	4.883071	-3.406299

Table S13. Cartesian coordinates for **E-gs**.

Pt1	8.031880	-1.178604	0.223280
Cl2	10.407838	-1.235907	0.333588
Cl3	7.946197	-3.558692	0.460760
N4	7.914401	0.843341	0.011746
C5	7.509639	3.593910	-0.289854
C6	8.981927	1.688110	-0.015710
C7	6.632073	1.342951	-0.109554
C8	6.409999	2.718902	-0.261234
C9	8.811175	3.068998	-0.165469
N10	6.023433	-0.970329	0.108218
C11	3.271177	-0.468783	-0.117817
C12	5.569925	0.325371	-0.061190
C13	5.132791	-1.998732	0.188187
C14	3.758719	-1.781945	0.080683
C15	4.197113	0.589673	-0.173496
C16	1.817523	-0.139318	-0.246045
N17	0.976819	-1.215480	-0.580226
O18	1.364808	1.018921	-0.076402
C19	-0.423786	-1.116656	-0.812588
C20	-3.228119	-1.004202	-1.336622
C21	-0.942075	-1.643290	-1.981359
C22	-1.315905	-0.535511	0.184949
C23	-2.708066	-0.475273	-0.108452
C24	-2.349341	-1.614768	-2.270926
C25	-0.897965	-0.057149	1.458620
N26	-3.635311	0.057779	0.771224
C27	-1.842324	0.472306	2.337081
C28	-3.202390	0.528260	1.959663
N29	-4.590601	-0.904205	-1.548075
C30	-2.916243	-2.142251	-3.466037
C31	-4.292215	-2.040184	-3.667392
C32	-5.102957	-1.416342	-2.688616
C33	7.340726	5.068149	-0.448239
O34	8.268893	5.885848	-0.478636
O35	6.008500	5.435440	-0.560367
Ru36	-5.615441	0.031134	0.036435
N37	-6.453442	1.127624	1.615481
C38	-7.571357	2.785187	3.594488
C39	-7.034556	0.592653	2.725515
C40	-6.419814	2.498352	1.471012
C41	-6.975445	3.341527	2.452024
C42	-7.599895	1.384471	3.733253
N43	-7.536644	-0.224544	-0.763667
C44	-10.140949	-0.744838	-1.690895
C45	-8.159655	-1.413275	-0.448120
C46	-8.199030	0.688431	-1.527410
C47	-9.495278	0.465157	-2.009220
C48	-9.463034	-1.688662	-0.903589
N49	-6.122669	-1.872848	0.759939
C50	-6.978460	-4.425490	1.574440
C51	-7.364454	-2.339390	0.384362
C52	-5.321401	-2.664422	1.526006
C53	-5.712412	-3.939985	1.953151
C54	-7.807210	-3.614704	0.783409
N55	-5.328458	2.003228	-0.622573
C56	-4.979512	4.715615	-1.279677
C57	-5.774458	2.986201	0.234730
C58	-4.718896	2.364977	-1.785607
C59	-4.528776	3.704362	-2.149026
C60	-5.606838	4.348175	-0.079026
H61	9.954576	1.219436	0.084813
H62	5.409790	3.123104	-0.355505

H63	9.671377	3.729431	-0.185496
H64	5.570765	-2.979793	0.342645
H65	3.103286	-2.639881	0.194567
H66	3.829402	1.601222	-0.302691
H67	1.425765	-2.055095	-0.931274
H68	-0.271514	-2.072032	-2.721989
H69	0.143858	-0.091668	1.744461
H70	-1.546559	0.848506	3.310189
H71	-3.948867	0.944501	2.625458
H72	-2.280782	-2.615683	-4.208910
H73	-4.757848	-2.431973	-4.565251
H74	-6.173195	-1.327619	-2.830532
H75	5.918476	6.410121	-0.664490
H76	-6.949432	4.418118	2.331031
H77	-8.051058	0.912646	4.599534
H78	-8.003126	3.426770	4.355992
H79	-7.670236	1.606490	-1.750887
H80	-9.982576	1.221959	-2.614528
H81	-9.948619	-2.623373	-0.648968
H82	-11.146375	-0.947082	-2.046070
H83	-4.356267	-2.254944	1.795979
H84	-5.040419	-4.533455	2.563751
H85	-8.783225	-3.977693	0.483185
H86	-7.311011	-5.410285	1.886753
H87	-7.037586	-0.487687	2.796520
H88	-4.385507	1.559109	-2.426963
H89	-4.037833	3.943558	-3.086184
H90	-5.956196	5.116610	0.600517
H91	-4.845076	5.763023	-1.530219

Table S14. Cartesian coordinates for **E-aq**.

Pt1	8.056808	-1.035647	0.171012
Cl2	10.459152	-0.845302	0.544127
Cl3	8.276687	-3.467226	0.207598
N4	7.723245	0.967165	0.135230
C5	7.029656	3.673516	0.040923
C6	8.680297	1.921445	0.292223
C7	6.409438	1.334280	-0.067296
C8	6.043182	2.685904	-0.118209
C9	8.365058	3.283170	0.250157
N10	6.048331	-1.038143	-0.130710
C11	3.281340	-0.792199	-0.526390
C12	5.471630	0.212283	-0.214204
C13	5.273727	-2.147580	-0.249914
C14	3.890069	-2.059609	-0.446995
C15	4.094413	0.349774	-0.417840
C16	1.806411	-0.569049	-0.757189
N17	0.958529	-1.596895	-0.419247
O18	1.392025	0.528811	-1.222980
C19	-0.463615	-1.539803	-0.634653
C20	-3.269587	-1.459040	-1.056083
C21	-1.040652	-2.370244	-1.567699
C22	-1.272924	-0.637236	0.165549
C23	-2.674116	-0.607683	-0.067629
C24	-2.462743	-2.357511	-1.801906
C25	-0.758044	0.204282	1.189473
N26	-3.531348	0.210323	0.645021
C27	-1.632203	1.026322	1.898237
C28	-3.014120	1.012696	1.598418
N29	-4.636348	-1.362659	-1.232175
C30	-3.105724	-3.188321	-2.760345

C31	-4.486518	-3.085065	-2.927301
C32	-5.224063	-2.162427	-2.147849
C33	6.699386	5.129747	-0.006560
O34	7.534660	6.041958	0.126753
O35	5.361627	5.356881	-0.215905
Ru36	-5.544368	0.035047	0.051505
N37	-6.262807	1.567900	1.280373
C38	-7.223813	3.764189	2.744461
C39	-6.780050	1.396466	2.527562
C40	-6.216528	2.833933	0.738634
C41	-6.694016	3.944740	1.457573
C42	-7.266403	2.466949	3.288602
N43	-7.507843	-0.376581	-0.538988
C44	-10.165493	-1.060132	-1.141638
C45	-8.131314	-1.398594	0.143234
C46	-8.194582	0.294355	-1.503842
C47	-9.519227	-0.018917	-1.833466
C48	-9.461730	-1.753375	-0.144984
N49	-6.037301	-1.552225	1.326799
C50	-6.885710	-3.720000	2.898523
C51	-7.305738	-2.065976	1.169309
C52	-5.204128	-2.107633	2.248793
C53	-5.591917	-3.187516	3.051813
C54	-7.747014	-3.151871	1.947443
N55	-5.264569	1.712750	-1.171202
C56	-4.912505	4.097505	-2.613091
C57	-5.640790	2.917275	-0.618374
C58	-4.723172	1.694012	-2.419719
C59	-4.533490	2.861622	-3.169573
C60	-5.470953	4.121362	-1.325898
H61	9.689772	1.566527	0.450226
H62	5.014046	2.978293	-0.278278
H63	9.145623	4.023901	0.377281
H64	5.784646	-3.098992	-0.185175
H65	3.336461	-2.985365	-0.556097
H66	3.633867	1.326622	-0.496244
H67	1.334254	-2.460804	-0.042814
H68	-0.418341	-3.041920	-2.151570
H69	0.300229	0.200041	1.421067
H70	-1.272422	1.679818	2.684608
H71	-3.705020	1.644222	2.142012
H72	-2.523478	-3.888239	-3.351550
H73	-5.013031	-3.699935	-3.648204
H74	-6.295210	-2.066768	-2.270788
H75	5.139552	6.315697	-0.250137
H76	-6.656882	4.936678	1.024456
H77	-7.666951	2.281066	4.278756
H78	-7.594093	4.614470	3.307458
H79	-7.665669	1.087224	-2.015680
H80	-10.024073	0.543111	-2.611104
H81	-9.946214	-2.555440	0.398105
H82	-11.191952	-1.325752	-1.371677
H83	-4.218683	-1.670248	2.339482
H84	-4.893722	-3.594972	3.774251
H85	-8.744753	-3.552254	1.816143
H86	-7.215962	-4.557199	3.504395
H87	-6.795912	0.385489	2.912273
H88	-4.447802	0.725484	-2.815631
H89	-4.099903	2.796321	-4.161128
H90	-5.765729	5.065123	-0.883752
H91	-4.776835	5.020187	-3.167476

Table S15. Cartesian coordinates for **F-gs**.

Pt1	8.031570	-1.178854	0.223505
Cl2	10.407510	-1.236782	0.333930
Cl3	7.945267	-3.558827	0.461319
N4	7.914480	0.843071	0.011660
C5	7.510210	3.593692	-0.290174
C6	8.982152	1.687654	-0.015806
C7	6.632247	1.342901	-0.109754
C8	6.410416	2.718879	-0.261560
C9	8.811646	3.068562	-0.165679
N10	6.023192	-0.970235	0.108280
C11	3.271051	-0.468292	-0.118109
C12	5.569922	0.325511	-0.061339
C13	5.132383	-1.998500	0.188282
C14	3.758365	-1.781516	0.080629
C15	4.197157	0.590014	-0.173827
C16	1.817464	-0.138672	-0.246496
N17	0.976783	-1.214727	-0.581284
O18	1.364722	1.019478	-0.076509
C19	-0.423828	-1.115908	-0.813473
C20	-3.228253	-1.003552	-1.337151
C21	-0.942206	-1.642181	-1.982365
C22	-1.315902	-0.535160	0.184350
C23	-2.708097	-0.474939	-0.108877
C24	-2.349514	-1.613721	-2.271746
C25	-0.897842	-0.057160	1.458119
N26	-3.635274	0.057782	0.771081
C27	-1.842131	0.471949	2.336862
C28	-3.202244	0.527923	1.959612
N29	-4.590769	-0.903676	-1.548407
C30	-2.916487	-2.140915	-3.466951
C31	-4.292498	-2.038962	-3.668112
C32	-5.103202	-1.415541	-2.689037
C33	7.341563	5.067951	-0.448661
O34	8.269872	5.885485	-0.479094
O35	6.009403	5.435455	-0.560916
Ru36	-5.615494	0.031152	0.036491
N37	-6.453260	1.127173	1.615963
C38	-7.570764	2.784170	3.595675
C39	-7.034346	0.591879	2.725857
C40	-6.419452	2.497951	1.471988
C41	-6.974885	3.340844	2.453355
C42	-7.599481	1.383408	3.733935
N43	-7.536688	-0.224466	-0.763578
C44	-10.140831	-0.744778	-1.691231
C45	-8.159595	-1.413358	-0.448446
C46	-8.199110	0.688691	-1.527077
C47	-9.495279	0.465408	-2.009091
C48	-9.462891	-1.688763	-0.904140
N49	-6.122630	-1.873018	0.759565
C50	-6.978239	-4.425864	1.573593
C51	-7.364362	-2.339593	0.383864
C52	-5.321310	-2.664662	1.525513
C53	-5.712234	-3.940334	1.952416
C54	-7.807033	-3.615004	0.782686
N55	-5.328528	2.003440	-0.621978
C56	-4.979117	4.716026	-1.278023
C57	-5.774172	2.986158	0.235807
C58	-4.719135	2.365540	-1.784990
C59	-4.528800	3.705034	-2.147893
C60	-5.606289	4.348224	-0.077403
H61	9.954715	1.218822	0.084808
H62	5.410288	3.123256	-0.355935

H63	9.671964	3.728845	-0.185720
H64	5.570224	-2.979601	0.342899
H65	3.102747	-2.639296	0.194597
H66	3.829636	1.601604	-0.303250
H67	1.425804	-2.054078	-0.932884
H68	-0.271708	-2.070605	-2.723238
H69	0.144009	-0.091714	1.743844
H70	-1.546290	0.847858	3.310060
H71	-3.948658	0.943885	2.625651
H72	-2.281046	-2.614020	-4.210048
H73	-4.758185	-2.430534	-4.566037
H74	-6.173475	-1.326950	-2.830763
H75	5.919549	6.410141	-0.665149
H76	-6.948748	4.417475	2.332748
H77	-8.050626	0.911333	4.600090
H78	-8.002368	3.425538	4.357454
H79	-7.670406	1.606899	-1.750167
H80	-9.982610	1.222341	-2.614208
H81	-9.948373	-2.623621	-0.649856
H82	-11.146184	-0.947045	-2.046598
H83	-4.356217	-2.255150	1.795574
H84	-5.040215	-4.533864	2.562929
H85	-8.783030	-3.977998	0.482400
H86	-7.310732	-5.410735	1.885733
H87	-7.037504	-0.488484	2.796470
H88	-4.386058	1.559861	-2.426743
H89	-4.038018	3.944510	-3.085064
H90	-5.955319	5.116450	0.602545
H91	-4.844473	5.763508	-1.528141

Table S16. Cartesian coordinates for **F-aq**.

Pt1	8.024911	-1.173537	0.274705
Cl2	10.464915	-1.246286	0.334245
Cl3	7.983872	-3.591735	0.586277
N4	7.905096	0.832097	-0.013273
C5	7.504342	3.564411	-0.442953
C6	8.971383	1.674553	-0.078221
C7	6.624687	1.325278	-0.157655
C8	6.404929	2.692135	-0.374622
C9	8.803707	3.046456	-0.291388
N10	6.005510	-0.968282	0.179917
C11	3.260643	-0.465107	-0.079192
C12	5.560576	0.315644	-0.057723
C13	5.110736	-1.980847	0.316212
C14	3.733492	-1.763054	0.194263
C15	4.192660	0.582211	-0.187575
C16	1.801031	-0.123100	-0.237678
N17	0.973727	-1.155277	-0.626488
O18	1.385430	1.050749	-0.036735
C19	-0.430157	-1.003630	-0.883930
C20	-3.205155	-0.760342	-1.442273
C21	-0.908732	-1.291208	-2.143666
C22	-1.333572	-0.606586	0.183265
C23	-2.715619	-0.475997	-0.124655
C24	-2.309882	-1.189357	-2.455915
C25	-0.936692	-0.370006	1.528153
N26	-3.658133	-0.104303	0.816806
C27	-1.896747	0.002647	2.467176
C28	-3.249502	0.137960	2.079445
N29	-4.560530	-0.608784	-1.660812
C30	-2.848815	-1.477840	-3.740340

C31	-4.219583	-1.328112	-3.947537
C32	-5.049341	-0.891538	-2.887356
C33	7.330899	5.030595	-0.671656
O34	8.268824	5.845257	-0.736536
O35	6.011780	5.387260	-0.804240
Ru36	-5.613352	0.023402	0.044706
N37	-6.476597	0.811617	1.780953
C38	-7.625844	2.078687	4.009222
C39	-7.074680	0.081258	2.761559
C40	-6.440238	2.184391	1.891269
C41	-7.011199	2.835416	2.999973
C42	-7.656789	0.676927	3.887549
N43	-7.509441	-0.058767	-0.832912
C44	-10.083752	-0.372238	-1.911947
C45	-8.149019	-1.276565	-0.753587
C46	-8.138917	0.985264	-1.438030
C47	-9.421404	0.867119	-1.988464
C48	-9.438179	-1.451071	-1.288675
N49	-6.147269	-1.972858	0.394433
C50	-7.047230	-4.613714	0.722670
C51	-7.384422	-2.346397	-0.082751
C52	-5.368503	-2.897793	1.019478
C53	-5.783191	-4.222887	1.202921
C54	-7.851644	-3.664274	0.074016
N55	-5.311074	2.077932	-0.235730
C56	-4.962458	4.861289	-0.384789
C57	-5.774147	2.888127	0.777544
C58	-4.685758	2.641909	-1.305171
C59	-4.495269	4.025030	-1.415939
C60	-5.606909	4.283790	0.719906
H61	9.946588	1.222160	0.041940
H62	5.403403	3.084852	-0.489095
H63	9.668741	3.697276	-0.338925
H64	5.522485	-2.960064	0.520847
H65	3.068812	-2.607130	0.338688
H66	3.831848	1.586272	-0.372534
H67	1.395922	-2.023468	-0.940548
H68	-0.220150	-1.589695	-2.928859
H69	0.098421	-0.483157	1.824456
H70	-1.625123	0.190124	3.499650
H71	-4.005862	0.429122	2.796798
H72	-2.196087	-1.807436	-4.542652
H73	-4.669021	-1.538529	-4.911258
H74	-6.114183	-0.764792	-3.034726
H75	5.892586	6.353118	-0.954743
H76	-6.980854	3.915147	3.078733
H77	-8.120550	0.053065	4.643289
H78	-8.069268	2.570815	4.868440
H79	-7.596928	1.920605	-1.480115
H80	-9.881904	1.727034	-2.461660
H81	-9.935369	-2.411017	-1.222801
H82	-11.078233	-0.496422	-2.327472
H83	-4.405746	-2.559629	1.379255
H84	-5.128221	-4.923268	1.708779
H85	-8.825844	-3.950277	-0.303074
H86	-7.397883	-5.632565	0.849484
H87	-7.076783	-0.993156	2.635117
H88	-4.344247	1.967983	-2.079585
H89	-3.993174	4.427872	-2.288310
H90	-5.970924	4.914693	1.521402
H91	-4.829150	5.936611	-0.439235

Table S17. Cartesian coordinates for **G-gs**.

Pt1	-8.062523	-1.068982	-0.006728
Cl2	-10.429378	-0.870023	0.131104
Cl3	-8.261283	-3.436117	-0.257601
N4	-7.714311	0.925866	0.189748
C5	-7.000229	3.619319	0.435458
C6	-8.679882	1.875523	0.339602
C7	-6.382316	1.290928	0.160749
C8	-6.007813	2.636217	0.282854
C9	-8.354389	3.230410	0.464403
N10	-6.039401	-1.072956	-0.099389
C11	-3.243087	-0.851715	-0.217270
C12	-5.442491	0.169322	-0.004751
C13	-5.268454	-2.191481	-0.235223
C14	-3.877453	-2.112129	-0.292899
C15	-4.044741	0.296587	-0.062565
C16	-1.748809	-0.833147	-0.282603
N17	-1.140460	0.395331	-0.607071
O18	-1.056996	-1.858303	-0.073782
C19	0.261675	0.532782	-0.822142
C20	3.058498	0.737016	-1.345657
C21	0.713459	1.077943	-2.009052
C22	1.213858	0.125269	0.204196
C23	2.602645	0.208689	-0.092274
C24	2.116129	1.212173	-2.296898
C25	0.850498	-0.327543	1.503330
N26	3.583340	-0.183004	0.803240
C27	1.847378	-0.702468	2.402607
C28	3.205144	-0.635424	2.016926
N29	4.423120	0.767586	-1.565524
C30	2.620495	1.755265	-3.512774
C31	3.999296	1.795455	-3.718362
C32	4.874638	1.291423	-2.726285
C33	-6.663281	5.065367	0.568590
O34	-7.488768	5.975305	0.711312
O35	-5.293664	5.298104	0.514336
Ru36	5.542984	-0.034263	0.027264
N37	6.483205	-1.014909	1.626338
C38	7.744104	-2.520371	3.640442
C39	7.050186	-0.401723	2.702629
C40	6.534325	-2.389360	1.533961
C41	7.162454	-3.156982	2.533076
C42	7.684845	-1.116372	3.726587
N43	7.426941	0.316411	-0.821470
C44	9.978360	0.968114	-1.811242
C45	7.980489	1.550090	-0.551789
C46	8.131677	-0.576273	-1.570944
C47	9.403340	-0.287953	-2.083094
C48	9.256537	1.891398	-1.038625
N49	5.936930	1.920578	0.675411
C50	6.644792	4.544229	1.400410
C51	7.142374	2.450435	0.266777
C52	5.097751	2.684931	1.428226
C53	5.415319	3.994390	1.811085
C54	7.511540	3.761857	0.621588
N55	5.370610	-2.047733	-0.551892
C56	5.170767	-4.801412	-1.088744
C57	5.894699	-2.965488	0.333061
C58	4.758102	-2.493887	-1.683568
C59	4.640006	-3.856442	-1.986873
C60	5.802766	-4.346973	0.079298
H61	-9.700266	1.508477	0.354317
H62	-4.968566	2.939451	0.264330

H63	-9.135501	3.973682	0.582291
H64	-5.814252	-3.127422	-0.293957
H65	-3.283829	-3.013553	-0.393495
H66	-3.606626	1.282847	0.052102
H67	-1.730354	1.118749	-1.004792
H68	-0.000515	1.378386	-2.772005
H69	-0.189656	-0.387608	1.793218
H70	1.595893	-1.056411	3.396291
H71	3.992433	-0.940682	2.695789
H72	1.936264	2.127956	-4.269591
H73	4.417947	2.203161	-4.632138
H74	5.947488	1.304681	-2.875490
H75	-5.102925	6.259452	0.607346
H76	7.202851	-4.236905	2.452963
H77	8.121322	-0.583787	4.564707
H78	8.231181	-3.103573	4.415410
H79	7.657484	-1.531555	-1.757594
H80	9.926176	-1.031025	-2.675633
H81	9.687786	2.861083	-0.819237
H82	10.963366	1.220900	-2.190412
H83	4.163376	2.224800	1.724009
H84	4.716106	4.564348	2.413466
H85	8.460006	4.173736	0.297096
H86	6.920707	5.556140	1.679456
H87	6.984494	0.678500	2.733265
H88	4.362152	-1.737394	-2.349056
H89	4.141690	-4.164010	-2.899856
H90	6.212476	-5.064220	0.780777
H91	5.092430	-5.864636	-1.292014

Table S18. Cartesian coordinates for **G-aq**.

Pt1	-8.092384	-1.088716	0.239486
Cl2	-10.525695	-0.895785	0.297873
Cl3	-8.307698	-3.470031	0.735099
N4	-7.760462	0.879927	-0.121433
C5	-7.066744	3.555389	-0.538690
C6	-8.731930	1.824747	-0.242113
C7	-6.431795	1.239589	-0.214992
C8	-6.065790	2.576445	-0.420807
C9	-8.417242	3.170990	-0.452201
N10	-6.063349	-1.107740	0.113401
C11	-3.280521	-0.898619	-0.127883
C12	-5.482416	0.123195	-0.095043
C13	-5.286088	-2.221894	0.189218
C14	-3.896051	-2.150941	0.058040
C15	-4.089644	0.248067	-0.205584
C16	-1.785952	-0.844494	-0.323376
N17	-1.135630	0.200348	0.294644
O18	-1.198638	-1.721822	-1.012335
C19	0.250346	0.531191	0.108233
C20	2.968793	1.264320	-0.268124
C21	0.568521	1.791336	-0.350387
C22	1.292842	-0.422745	0.448088
C23	2.644801	-0.041637	0.227544
C24	1.936015	2.199458	-0.536521
C25	1.058587	-1.705449	1.016907
N26	3.710767	-0.879026	0.502955
C27	2.142171	-2.535445	1.298024
C28	3.457636	-2.099882	1.017144
N29	4.305980	1.558396	-0.451885
C30	2.312421	3.490268	-1.001108

C31	3.665681	3.779436	-1.172240
C32	4.638952	2.791330	-0.890068
C33	-6.735289	4.996098	-0.753920
O34	-7.582118	5.900348	-0.866157
O35	-5.381654	5.218500	-0.814216
Ru36	5.583310	-0.040449	0.024856
N37	6.693326	-1.778392	0.375879
C38	8.182156	-4.148230	0.619351
C39	7.303348	-2.096205	1.550248
C40	6.813260	-2.633367	-0.697756
C41	7.555331	-3.824034	-0.593546
C42	8.052267	-3.268789	1.710419
N43	7.360733	0.997932	-0.340548
C44	9.756037	2.440419	-0.610709
C45	7.860888	1.714002	0.725041
C46	8.042067	0.995626	-1.518858
C47	9.238034	1.703563	-1.692165
C48	9.058646	2.442208	0.607078
N49	5.931282	0.856088	1.887364
C50	6.556754	2.199431	4.273656
C51	7.056196	1.647835	1.960914
C52	5.131079	0.733917	2.981602
C53	5.410891	1.386427	4.188854
C54	7.384057	2.328632	3.147650
N55	5.471075	-0.989025	-1.840224
C56	5.407200	-2.454540	-4.236296
C57	6.117823	-2.202366	-1.926576
C58	4.803716	-0.512819	-2.926611
C59	4.750729	-1.213504	-4.138092
C60	6.095829	-2.949774	-3.118288
H61	-9.752502	1.474999	-0.163745
H62	-5.025880	2.866724	-0.489314
H63	-9.209563	3.904476	-0.543668
H64	-5.804579	-3.157495	0.350885
H65	-3.305634	-3.058414	0.101003
H66	-3.651942	1.221982	-0.388900
H67	-1.685189	0.852867	0.845805
H68	-0.223482	2.494563	-0.591835
H69	0.049896	-2.034623	1.229812
H70	1.995530	-3.518222	1.731039
H71	4.309407	-2.735809	1.221514
H72	1.551924	4.233714	-1.218367
H73	3.993020	4.751528	-1.522976
H74	5.692780	2.997292	-1.026994
H75	-5.158030	6.167032	-0.956017
H76	7.646878	-4.490534	-1.442364
H77	8.518717	-3.479352	2.666231
H78	8.757181	-5.063756	0.710117
H79	7.612335	0.419708	-2.327676
H80	9.743792	1.672648	-2.650657
H81	9.446156	3.002471	1.449055
H82	10.680374	2.999359	-0.712113
H83	4.261965	0.097910	2.878314
H84	4.744402	1.256935	5.034118
H85	8.268902	2.951161	3.197460
H86	6.800874	2.719762	5.193878
H87	7.179288	-1.397235	2.366529
H88	4.315080	0.445992	-2.815960
H89	4.207764	-0.791942	-4.976481
H90	6.605778	-3.903373	-3.178300
H91	5.384313	-3.022744	-5.160247

Table S19. Cartesian coordinates for **H-gs**.

Pt1	-8.062412	-1.069000	-0.006637
Cl2	-10.429255	-0.870112	0.131597
Cl3	-8.261129	-3.436157	-0.257427
N4	-7.714246	0.925857	0.189815
C5	-7.000198	3.619340	0.435363
C6	-8.679820	1.875495	0.339806
C7	-6.382267	1.290956	0.160631
C8	-6.007784	2.636261	0.282618
C9	-8.354341	3.230390	0.464540
N10	-6.039300	-1.072924	-0.099575
C11	-3.242990	-0.851564	-0.217728
C12	-5.442424	0.169377	-0.004965
C13	-5.268322	-2.191394	-0.235580
C14	-3.877325	-2.111984	-0.293404
C15	-4.044691	0.296692	-0.062880
C16	-1.748726	-0.832966	-0.283135
N17	-1.140365	0.395593	-0.607391
O18	-1.056892	-1.858145	-0.074512
C19	0.261798	0.533000	-0.822408
C20	3.058648	0.737288	-1.345653
C21	0.713672	1.078355	-2.009185
C22	1.213882	0.125328	0.203957
C23	2.602689	0.208748	-0.092391
C24	2.116378	1.212608	-2.296899
C25	0.850397	-0.327578	1.503025
N26	3.583302	-0.183093	0.803148
C27	1.847193	-0.702645	2.402330
C28	3.204994	-0.635630	2.016755
N29	4.423292	0.767914	-1.565385
C30	2.620850	1.755930	-3.512623
C31	3.999673	1.796184	-3.718071
C32	4.874922	1.291983	-2.725999
C33	-6.663282	5.065406	0.568391
O34	-7.488782	5.975308	0.711250
O35	-5.293682	5.298189	0.513981
Ru36	5.543008	-0.034284	0.027303
N37	6.483015	-1.015351	1.626247
C38	7.743262	-2.521378	3.640322
C39	7.050077	-0.402433	2.702640
C40	6.533765	-2.389806	1.533714
C41	7.161555	-3.157713	2.532826
C42	7.684428	-1.117368	3.726591
N43	7.427006	0.316522	-0.821236
C44	9.978490	0.968299	-1.810758
C45	7.980559	1.550147	-0.551351
C46	8.131750	-0.576078	-1.570809
C47	9.403454	-0.287711	-2.082835
C48	9.256648	1.891494	-1.038052
N49	5.937000	1.920381	0.675913
C50	6.644792	4.543953	1.401306
C51	7.142419	2.450355	0.267332
C52	5.097835	2.684577	1.428901
C53	5.415382	3.993981	1.811980
C54	7.511526	3.761748	0.622295
N55	5.370434	-2.047619	-0.552271
C56	5.170094	-4.801202	-1.089526
C57	5.894159	-2.965616	0.332646
C58	4.758072	-2.493503	-1.684135
C59	4.639745	-3.855989	-1.987644
C60	5.801950	-4.347051	0.078704
H61	-9.700190	1.508421	0.354681
H62	-4.968550	2.939527	0.263897

H63	-9.135454	3.973641	0.582551
H64	-5.814068	-3.127363	-0.294316
H65	-3.283698	-3.013388	-0.394154
H66	-3.606643	1.282981	0.051802
H67	-1.730202	1.118979	-1.005251
H68	-0.000220	1.378950	-2.772154
H69	-0.189784	-0.387592	1.792827
H70	1.595628	-1.056687	3.395958
H71	3.992207	-0.940995	2.695658
H72	1.936687	2.128781	-4.269423
H73	4.418408	2.204099	-4.631714
H74	5.947791	1.305315	-2.875060
H75	-5.102958	6.259543	0.606955
H76	7.201650	-4.237641	2.452618
H77	8.121013	-0.584993	4.564788
H78	8.230078	-3.104803	4.415286
H79	7.657522	-1.531303	-1.757663
H80	9.926297	-1.030689	-2.675487
H81	9.687893	2.861151	-0.818525
H82	10.963505	1.221135	-2.189874
H83	4.163484	2.224376	1.724647
H84	4.716183	4.563798	2.414510
H85	8.459940	4.173732	0.297779
H86	6.920670	5.555838	1.680481
H87	6.984700	0.677806	2.733372
H88	4.362417	-1.736847	-2.349610
H89	4.141598	-4.163312	-2.900802
H90	6.211358	-5.064467	0.780184
H91	5.091571	-5.864381	-1.292959

Table S20. Cartesian coordinates for **H-aq**.

Pt1	-8.109477	-0.872360	-0.020150
Cl2	-10.500687	-0.413546	0.101833
Cl3	-8.637542	-3.229502	-0.338198
N4	-7.530694	1.052542	0.258657
C5	-6.510012	3.627008	0.633182
C6	-8.376907	2.096064	0.472172
C7	-6.167666	1.263174	0.225560
C8	-5.638445	2.547314	0.411866
C9	-7.897401	3.395721	0.663425
N10	-6.095033	-1.107026	-0.134830
C11	-3.301393	-1.185080	-0.333286
C12	-5.364499	0.054209	-0.011565
C13	-5.457612	-2.292757	-0.332252
C14	-4.065214	-2.363874	-0.427452
C15	-3.965523	0.034348	-0.112516
C16	-1.802393	-1.295299	-0.437786
N17	-1.149848	-0.209825	-0.983436
O18	-1.200300	-2.334784	-0.054809
C19	0.271269	-0.164062	-1.187630
C20	3.073621	-0.040572	-1.630233
C21	0.762429	-0.082524	-2.471755
C22	1.167475	-0.155129	-0.043898
C23	2.566484	-0.104294	-0.290268
C24	2.177107	-0.008644	-2.729619
C25	0.739323	-0.160897	1.311961
N26	3.502763	-0.084132	0.727118
C27	1.693198	-0.138199	2.327891
C28	3.069322	-0.107943	2.004436
N29	4.445471	-0.001857	-1.786321
C30	2.731468	0.075081	-4.036831

C31	4.117634	0.119809	-4.182087
C32	4.948236	0.079475	-3.036822
C33	-6.001576	5.016802	0.837873
O34	-6.728405	6.006992	1.034487
O35	-4.631176	5.085530	0.785124
Ru36	5.491165	-0.040120	0.037043
N37	6.368470	-0.251112	1.925280
C38	7.560197	-0.760012	4.417725
C39	6.787362	0.774843	2.715659
C40	6.537400	-1.547769	2.359498
C41	7.132512	-1.820723	3.604589
C42	7.383694	0.560698	3.964738
N43	7.393840	0.168891	-0.804312
C44	9.939942	0.671677	-1.878932
C45	7.817378	1.465114	-1.001943
C46	8.221212	-0.859523	-1.136612
C47	9.496414	-0.648468	-1.675883
C48	9.089850	1.734831	-1.537885
N49	5.665645	2.043982	-0.082909
C50	6.087357	4.804981	-0.379230
C51	6.847497	2.509393	-0.616435
C52	4.708135	2.935373	0.292668
C53	4.882564	4.318845	0.162081
C54	7.075531	3.889075	-0.771553
N55	5.541200	-2.124750	0.241977
C56	5.638227	-4.885002	0.751175
C57	6.059416	-2.590600	1.430206
C58	5.081652	-3.015654	-0.678756
C59	5.114901	-4.398886	-0.461537
C60	6.114410	-3.969706	1.702493
H61	-9.432826	1.861274	0.483900
H62	-4.571001	2.721476	0.388911
H63	-8.591753	4.210319	0.832018
H64	-6.088389	-3.167737	-0.414319
H65	-3.582943	-3.322322	-0.577661
H66	-3.408235	0.955690	0.005379
H67	-1.698762	0.512712	-1.439384
H68	0.077246	-0.087123	-3.314648
H69	-0.316075	-0.172308	1.554475
H70	1.399153	-0.140279	3.371206
H71	3.821784	-0.089661	2.782315
H72	2.078804	0.101390	-4.903831
H73	4.578584	0.183599	-5.161098
H74	6.026029	0.106411	-3.133435
H75	-4.290749	5.999775	0.919351
H76	7.264218	-2.842460	3.938634
H77	7.699605	1.410367	4.559443
H78	8.020090	-0.959674	5.379869
H79	7.844407	-1.859537	-0.968210
H80	10.119127	-1.499970	-1.926053
H81	9.418198	2.755931	-1.687678
H82	10.923203	0.869079	-2.292813
H83	3.796880	2.524326	0.706647
H84	4.091756	4.990176	0.477271
H85	8.006045	4.249021	-1.193073
H86	6.253617	5.870953	-0.493938
H87	6.633573	1.775820	2.335109
H88	4.690700	-2.604127	-1.599894
H89	4.738318	-5.069872	-1.225308
H90	6.520395	-4.329617	2.639863
H91	5.675746	-5.950649	0.951400

Table S21. Cartesian coordinates for **I-gs**.

Pt1	-8.020407	-1.117304	-0.010537
Cl2	-10.392943	-1.137295	0.168931
Cl3	-8.004284	-3.490284	-0.320649
N4	-7.845118	0.896520	0.235454
C5	-7.361888	3.634137	0.544498
C6	-8.886542	1.753595	0.423470
C7	-6.550800	1.377570	0.198706
C8	-6.289403	2.746631	0.350640
C9	-8.676290	3.128103	0.581420
N10	-6.009376	-0.938435	-0.137931
C11	-3.246919	-0.469264	-0.294613
C12	-5.519579	0.348591	-0.009132
C13	-5.149323	-1.978517	-0.328558
C14	-3.770700	-1.777949	-0.411370
C15	-4.141070	0.595958	-0.079711
C16	-1.785296	-0.159520	-0.354060
N17	-0.976691	-1.128758	-0.973052
O18	-1.294318	0.897878	0.112398
C19	0.426793	-0.981271	-1.164597
C20	3.229704	-0.675604	-1.600910
C21	0.953174	-1.096497	-2.436767
C22	1.308174	-0.753510	-0.026035
C23	2.697654	-0.572812	-0.272594
C24	2.363000	-0.964272	-2.689192
C25	0.876864	-0.729191	1.329626
N26	3.608676	-0.316803	0.738344
C27	1.807993	-0.497897	2.340841
C28	3.165145	-0.281242	2.012519
N29	4.591867	-0.499473	-1.756847
C30	2.942655	-1.073443	-3.985141
C31	4.317954	-0.894281	-4.131670
C32	5.115355	-0.605694	-2.997990
C33	-7.150956	5.101806	0.712051
O34	-8.053702	5.929617	0.887515
O35	-5.810379	5.451178	0.649413
Ru36	5.581931	-0.034691	0.045843
N37	6.435155	0.252258	1.938536
C38	7.650693	0.418889	4.469715
C39	6.622508	1.458571	2.542722
C40	6.850760	-0.893040	2.584001
C41	7.461424	-0.826606	3.850647
C42	7.221658	1.582261	3.802938
N43	7.438308	0.391715	-0.830191
C44	9.872117	1.188489	-1.995320
C45	7.604539	1.687916	-1.269541
C46	8.467235	-0.490775	-0.967307
C47	9.692746	-0.132723	-1.543535
C48	8.816228	2.102301	-1.854463
N49	5.358826	1.996382	-0.442870
C50	5.245663	4.686617	-1.256145
C51	6.439554	2.575289	-1.073032
C52	4.241804	2.744161	-0.221717
C53	4.148048	4.086874	-0.610194
C54	6.398694	3.920102	-1.487067
N55	6.023809	-2.007055	0.610365
C56	6.655409	-4.569703	1.582938
C57	6.606436	-2.152664	1.851402
C58	5.758925	-3.118092	-0.131920
C59	6.060615	-4.410384	0.316640
C60	6.928160	-3.428287	2.352825
H61	-9.871281	1.300037	0.440940
H62	-5.279326	3.135854	0.321285

H63	-9.516169	3.798138	0.730302
H64	-5.614329	-2.956403	-0.403614
H65	-3.137904	-2.652905	-0.523468
H66	-3.745388	1.599010	0.031179
H67	-1.441190	-1.831370	-1.539128
H68	0.289465	-1.261252	-3.281882
H69	-0.164261	-0.885259	1.577619
H70	1.504803	-0.474158	3.381745
H71	3.897833	-0.077731	2.784094
H72	2.317205	-1.290833	-4.846188
H73	4.792349	-0.969482	-5.104178
H74	6.184798	-0.461697	-3.094793
H75	-5.693849	6.422180	0.761393
H76	7.789079	-1.729917	4.351744
H77	7.348593	2.564771	4.244717
H78	8.120904	0.480657	5.445939
H79	8.292376	-1.497195	-0.608589
H80	10.482604	-0.870992	-1.631380
H81	8.941964	3.123528	-2.194491
H82	10.810456	1.498688	-2.443902
H83	3.418306	2.249637	0.277409
H84	3.237126	4.641287	-0.411797
H85	7.250016	4.368577	-1.985544
H86	5.204354	5.724084	-1.572248
H87	6.279439	2.329458	1.998744
H88	5.301818	-2.953548	-1.099605
H89	5.832688	-5.265487	-0.310640
H90	7.383203	-3.536840	3.330356
H91	6.899437	-5.557505	1.960623

Table S22. Cartesian coordinates for **l-aq**.

Pt1	-7.997382	-1.219861	0.025042
Cl2	-10.436078	-1.363886	0.056166
Cl3	-7.894212	-3.657525	-0.031841
N4	-7.934716	0.807511	0.139216
C5	-7.606706	3.574484	0.358601
C6	-9.024568	1.618122	0.217801
C7	-6.667033	1.350369	0.162711
C8	-6.483219	2.735225	0.272255
C9	-8.893408	3.006025	0.328381
N10	-5.985229	-0.942965	-0.030787
C11	-3.256956	-0.317185	-0.143962
C12	-5.575740	0.371616	0.055407
C13	-5.063919	-1.932123	-0.164845
C14	-3.693362	-1.652492	-0.232543
C15	-4.215383	0.698415	0.017373
C16	-1.804322	0.080938	-0.180964
N17	-0.986909	-0.683905	-0.983040
O18	-1.386422	1.073698	0.475473
C19	0.409505	-0.392776	-1.169038
C20	3.163598	0.168805	-1.565913
C21	0.841337	0.101914	-2.378514
C22	1.345521	-0.651878	-0.089864
C23	2.717890	-0.354208	-0.307071
C24	2.232672	0.392899	-2.613380
C25	0.982014	-1.204200	1.168596
N26	3.686013	-0.557576	0.658540
C27	1.969440	-1.413277	2.130042
C28	3.313365	-1.075249	1.847552
N29	4.514231	0.426018	-1.701261
C30	2.726790	0.912010	-3.841726

C31	4.090310	1.177831	-3.963908
C32	4.958459	0.924261	-2.875273
C33	-7.471578	5.057222	0.482222
O34	-8.431779	5.844173	0.561693
O35	-6.160103	5.463045	0.499924
Ru36	5.623049	-0.024094	0.028271
N37	6.591622	-0.684600	1.761006
C38	7.944953	-1.765132	3.973031
C39	6.883075	0.090078	2.841355
C40	6.967347	-2.010332	1.762290
C41	7.646714	-2.567320	2.860920
C42	7.554519	-0.413091	3.962820
N43	7.448154	0.702661	-0.689066
C44	9.861781	1.870064	-1.527816
C45	7.680477	2.043323	-0.472011
C46	8.399473	-0.044435	-1.313066
C47	9.613585	0.502234	-1.747171
C48	8.884002	2.643853	-0.884209
N49	5.505212	1.998694	0.565585
C50	5.532394	4.748811	1.138813
C51	6.589956	2.769186	0.208427
C52	4.451172	2.586096	1.195446
C53	4.429137	3.952989	1.499790
C54	6.620143	4.147842	0.487086
N55	5.970384	-2.038719	-0.431958
C56	6.488315	-4.771642	-0.822165
C57	6.605488	-2.768829	0.548382
C58	5.598301	-2.656730	-1.586062
C59	5.841190	-4.016346	-1.817927
C60	6.871626	-4.138819	0.370260
H61	-9.988544	1.128100	0.191960
H62	-5.491183	3.166412	0.290273
H63	-9.776795	3.630407	0.390852
H64	-5.448778	-2.941994	-0.215753
H65	-3.000791	-2.481337	-0.325663
H66	-3.885667	1.726372	0.102015
H67	-1.405163	-1.367038	-1.607125
H68	0.124900	0.291862	-3.172413
H69	-0.049099	-1.467422	1.373091
H70	1.726924	-1.834239	3.099034
H71	4.089910	-1.223032	2.586986
H72	2.046214	1.097959	-4.666717
H73	4.505405	1.576391	-4.882546
H74	6.019936	1.120123	-2.958069
H75	-6.064836	6.439704	0.582882
H76	7.941734	-3.609371	2.853643
H77	7.763073	0.242847	4.800467
H78	8.468511	-2.185191	4.825384
H79	8.172160	-1.090965	-1.465595
H80	10.340012	-0.132982	-2.241328
H81	9.061052	3.697535	-0.707024
H82	10.793291	2.323574	-1.849854
H83	3.622802	1.942721	1.460416
H84	3.567609	4.374800	2.005019
H85	7.475567	4.747570	0.201412
H86	5.545929	5.811028	1.359268
H87	6.564794	1.123067	2.798229
H88	5.106176	-2.043199	-2.328771
H89	5.528055	-4.463872	-2.754463
H90	7.368752	-4.707609	1.146348
H91	6.689616	-5.827434	-0.969881

Table S23. Cartesian coordinates for **J-gs**.

Pt1	8.053252	-1.090412	0.257433
Cl2	10.423542	-0.885059	0.285539
Cl3	8.238335	-3.444698	0.616547
N4	7.716306	0.892149	-0.051811
C5	7.015241	3.568857	-0.463716
C6	8.687698	1.840874	-0.165150
C7	6.385146	1.249605	-0.144067
C8	6.016867	2.586626	-0.348700
C9	8.368733	3.187330	-0.371514
N10	6.028498	-1.100757	0.205814
C11	3.232903	-0.896369	0.063967
C12	5.438578	0.129522	-0.010513
C13	5.251029	-2.211039	0.369121
C14	3.859473	-2.138359	0.310960
C15	4.040958	0.247586	-0.088367
C16	1.738833	-0.880616	0.000793
N17	1.145905	0.195281	-0.688864
O18	1.034587	-1.783211	0.513409
C19	-0.255027	0.262879	-0.945036
C20	-3.049468	0.288588	-1.512706
C21	-0.702098	0.378174	-2.247145
C22	-1.209352	0.220750	0.155576
C23	-2.597283	0.196363	-0.154575
C24	-2.104107	0.412217	-2.566297
C25	-0.847776	0.221706	1.531511
N26	-3.578949	0.104273	0.817934
C27	-1.846023	0.160458	2.502339
C28	-3.202754	0.086197	2.113956
N29	-4.413834	0.264311	-1.732447
C30	-2.604759	0.519028	-3.894875
C31	-3.983160	0.495610	-4.105566
C32	-4.861740	0.363587	-3.003352
C33	6.684842	5.006242	-0.680906
O34	7.515428	5.916921	-0.783845
O35	5.314828	5.229256	-0.759407
Ru36	-5.536671	0.014146	0.033868
N37	-6.510282	-0.071882	1.888002
C38	-7.859202	0.036781	4.354159
C39	-6.862210	-1.214911	2.540138
C40	-6.823757	1.146174	2.453082
C41	-7.499595	1.217600	3.685870
C42	-7.532413	-1.201801	3.770281
N43	-7.385586	-0.240205	-0.922526
C44	-9.836962	-0.810502	-2.179060
C45	-7.686373	-1.531764	-1.299635
C46	-8.290392	0.748754	-1.165880
C47	-9.520095	0.505144	-1.790825
C48	-8.909079	-1.833428	-1.928923
N49	-5.534511	-2.053463	-0.340144
C50	-5.711924	-4.782744	-0.996084
C51	-6.648236	-2.537634	-0.992569
C52	-4.526810	-2.913131	-0.021130
C53	-4.579072	-4.278837	-0.329537
C54	-6.752402	-3.900780	-1.328103
N55	-5.769627	2.050466	0.480689
C56	-6.152728	4.717340	1.288946
C57	-6.398192	2.328457	1.675897
C58	-5.335604	3.082269	-0.295465
C59	-5.509357	4.422818	0.071549
C60	-6.598117	3.657822	2.094470
H61	9.707185	1.479885	-0.084851
H62	4.978172	2.884405	-0.417535

H63	9.154373	3.930071	-0.458735
H64	5.792142	-3.135726	0.540957
H65	3.261115	-3.031056	0.452932
H66	3.606142	1.232061	-0.228405
H67	1.744242	0.751015	-1.291312
H68	0.014353	0.401905	-3.064571
H69	0.192486	0.264389	1.825227
H70	-1.596609	0.157112	3.557665
H71	-3.990082	0.010461	2.854398
H72	-1.917952	0.611931	-4.731245
H73	-4.398821	0.572220	-5.104479
H74	-5.934858	0.339099	-3.149882
H75	5.128069	6.185817	-0.898392
H76	-7.746383	2.177841	4.123422
H77	-7.790782	-2.138395	4.252585
H78	-8.380771	0.081314	5.304899
H79	-8.011679	1.746908	-0.852483
H80	-10.208310	1.325572	-1.963585
H81	-9.141552	-2.851022	-2.220134
H82	-10.782643	-1.033593	-2.662647
H83	-3.671897	-2.490819	0.491500
H84	-3.751463	-4.923899	-0.054719
H85	-7.628832	-4.275639	-1.843604
H86	-5.782533	-5.835271	-1.251394
H87	-6.593878	-2.147514	2.060274
H88	-4.846932	2.814214	-1.223799
H89	-5.148849	5.211099	-0.580577
H90	-7.092527	3.870139	3.035173
H91	-6.302601	5.745500	1.602603

Table S24. Cartesian coordinates for **J-aq**.

Pt1	8.093223	-0.914858	0.255814
Cl2	10.495276	-0.477413	0.222701
Cl3	8.579631	-3.279829	0.573790
N4	7.544906	1.018743	-0.021978
C5	6.561426	3.607504	-0.400468
C6	8.405222	2.070154	-0.095404
C7	6.186060	1.228810	-0.133329
C8	5.675377	2.519731	-0.323930
C9	7.944412	3.376965	-0.284345
N10	6.075466	-1.144482	0.199067
C11	3.281534	-1.232689	0.001365
C12	5.364763	0.013835	-0.026083
C13	5.417469	-2.326310	0.347434
C14	4.024471	-2.399866	0.261537
C15	3.966511	-0.012332	-0.132542
C16	1.781307	-1.343844	-0.080146
N17	1.147987	-0.447047	-0.915489
O18	1.160219	-2.221852	0.577953
C19	-0.273085	-0.441695	-1.126000
C20	-3.077435	-0.437582	-1.574068
C21	-0.770717	-0.735495	-2.376123
C22	-1.163276	-0.093764	-0.031525
C23	-2.563475	-0.120102	-0.273321
C24	-2.186487	-0.729685	-2.639116
C25	-0.727719	0.295960	1.264820
N26	-3.494862	0.172116	0.706092
C27	-1.676473	0.605225	2.237798
C28	-3.054500	0.524551	1.931594
N29	-4.449542	-0.426466	-1.731794
C30	-2.747382	-1.022820	-3.912943

C31	-4.134049	-1.010834	-4.060325
C32	-4.958523	-0.710136	-2.949885
C33	6.073292	5.005493	-0.598584
O34	6.813983	6.001841	-0.676525
O35	4.704618	5.074576	-0.684963
Ru36	-5.487325	0.020106	0.042596
N37	-6.361713	0.641277	1.837824
C38	-7.554132	1.684814	4.157359
C39	-6.784214	-0.186594	2.832246
C40	-6.527851	2.001906	1.978074
C41	-7.122211	2.541499	3.133282
C42	-7.381561	0.296507	4.003318
N43	-7.394886	-0.347874	-0.733811
C44	-9.940303	-1.053751	-1.689637
C45	-7.821158	-1.656327	-0.665181
C46	-8.221122	0.593763	-1.265842
C47	-9.495867	0.280080	-1.753636
C48	-9.092627	-2.027369	-1.139450
N49	-5.680685	-2.039397	0.374949
C50	-6.119179	-4.798840	0.661099
C51	-6.858906	-2.601402	-0.064649
C52	-4.737160	-2.835088	0.948620
C53	-4.920202	-4.214287	1.110002
C54	-7.094790	-3.981651	0.069756
N55	-5.516479	2.100094	-0.207751
C56	-5.606387	4.905714	-0.313284
C57	-6.042088	2.815315	0.845849
C58	-5.041567	2.768376	-1.294096
C59	-5.070166	4.165714	-1.383749
C60	-6.095716	4.220670	0.809470
H61	9.457067	1.836277	-0.000241
H62	4.610886	2.692582	-0.410191
H63	8.649833	4.197678	-0.338614
H64	6.032100	-3.197665	0.529458
H65	3.525720	-3.352879	0.391134
H66	3.425664	0.912883	-0.289789
H67	1.708485	0.104991	-1.557690
H68	-0.091096	-0.992661	-3.183399
H69	0.329098	0.361119	1.492928
H70	-1.377015	0.907737	3.234696
H71	-3.803015	0.745343	2.681735
H72	-2.099194	-1.251837	-4.753088
H73	-4.600169	-1.228500	-5.014470
H74	-6.036305	-0.692753	-3.049880
H75	4.377629	5.994554	-0.813498
H76	-7.249192	3.612049	3.236830
H77	-7.700678	-0.402115	4.768495
H78	-8.013851	2.090878	5.052266
H79	-7.843668	1.606907	-1.301455
H80	-10.117390	1.064873	-2.169840
H81	-9.421646	-3.057608	-1.081463
H82	-10.922802	-1.329402	-2.058203
H83	-3.831134	-2.348995	1.285141
H84	-4.140100	-4.806867	1.574422
H85	-8.022354	-4.417470	-0.280426
H86	-6.291245	-5.864577	0.769118
H87	-6.632559	-1.246914	2.679600
H88	-4.641262	2.164926	-2.097753
H89	-4.681145	4.653043	-2.270643
H90	-6.511177	4.776406	1.641038
H91	-5.642993	5.989352	-0.351521