Basic Data

Chapter 3

Table S3.1 FTIR data of K_2CrO_4, isolated $ZnCrO_4$ synthesized in bulk water and in water/AOT/n-heptane W/O microemulsion at different [water]/[AOT] mole ratio, ω.

Sample	*Appearance of peaks / cm^{-1}*	
K_2CrO_4	719, 881	
Bulk $ZnCrO_4$	719, 879, 955	
Nano $ZnCrO_4$	ω=5	723, 928
	ω=10	723, 899, 936
	ω=15	722, 896
	ω=20	721, 890

Table S3.2 Molar absorbance coefficient values of nanocolloidal dispersions of $ZnCrO_4$ at two absorbance peaks 370 nm and 273 nm at different ω values.

	10^3 x ε/ $mol^{-1}dm^3cm$	
ω	***At 273 nm***	***At 370 nm***
2	1.110	2.680
10	0.927	2.747
15	1.054	2.919
20	1.166	3.660

Chapter 5

Table S5.1: Optimised structural parameters of Cu_2O clusters

Clusters	Symmetry	Bond distances (d)/Å		Reported (d)/Å	Angles		Reported
$(Cu_2O)_1$	C_{2v}	$Cu_{2\,CUS}$ $O_{1\,CUS}^{2}$	1.765^{L}	(a) 1.75	∠$Cu_{2\,CUS}$ $O_{1\,CUS}^{2}$ $Cu_{3\,CUS}$	$90.9°^{L}$	(a) 87°
		$Cu_{3\,CUS}$ $O_{1\,CUS}^{2}$	1.788^{G}			$93.1°^{G}$	
		$Cu_{2\,CUS}$ $Cu_{3\,CUS}$	2.516^{L} 2.611^{G}	(a) 2.41	∠$O_{1\,CUS}^{2}$ $Cu_{2\,CUS}$ $Cu_{3\,CUS}$	$44.5°^{L}$ $43°^{G}$	
$(Cu_2O)_2$	C_{2v}	$Cu_{2\,CSA}$ $O_{1\,CUS}^{3}$	1.999^{L}	(b) 1.91	∠$Cu_{2\,CSA}$ $O_{1\,CUS}^{3}$ $Cu_{3\,CSA}$	$72.4°^{L}$	
		$Cu_{3\,CSA}$ $O_{1\,CUS}^{3}$	2.026^{G}		∠$Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$ $Cu_{3\,CSA}$	$74.2°^{G}$	
		$Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$			∠$O_{1\,CUS}^{3}$ $Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$	107.5^{L}	(b) 109.6°
		$Cu_{3\,CSA}$ $O_{4\,CUS}^{3}$			∠$O_{1\,CUS}^{3}$ $Cu_{3\,CSA}$ $O_{4\,CUS}^{3}$	105.3^{G}	
		$Cu_{6\,CUS}$ $O_{1\,CUS}^{3}$	1.830^{L}	(b) 1.76	∠$O_{1\,CUS}^{3}$ $Cu_{2\,CSA}$ Cu_{3CSA}	$53.8°^{L}$	
		$Cu_{5\,CUS}$ $O_{4\,CUS}^{3}$	1.830^{G}		∠$O_{1\,CUS}^{3}$ $Cu_{3\,CSA}$ Cu_{2CSA}	$52.9°^{G}$	
					∠$O_{4\,CUS}^{3}$ $Cu_{2\,CSA}$ Cu_{3CSA}		
					∠$O_{4\,CUS}^{3}$ $Cu_{3\,CSA}$ Cu_{2CSA}		
		$Cu_{2\,CSA}$ $Cu_{3\,CSA}$	2.361^{L} 2.445^{G}		∠$Cu_{2\,CSA}$ $O_{1\,CUS}^{3}$ $Cu_{6\,CUS}$	$82.6°^{L}$	
					∠$Cu_{3\,CSA}$ $O_{1\,CUS}^{3}$ $Cu_{6\,CUS}$	$87.4°^{G}$	
					∠$Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$ $Cu_{5\,CUS}$		
					∠$Cu_{3\,CSA}$ $O_{4\,CUS}^{3}$ $Cu_{5\,CUS}$		
$(Cu_2O)_3$	C_{2v}	$Cu_{2\,CSA}$ O_{1CSA} $Cu_{2\,CSA}$ $O_{4\,CSA}$	2.026^{L}		∠$Cu_{2\,CSA}$ $O_{1\,CSA}$ $Cu_{3\,CSA}$	$75.1°^{L}$	
		$Cu_{3\,CSA}$ $O_{1\,CSA}$ $Cu_{3\,CSA}$ $O_{4\,CSA}$	2.057^{G}		∠$Cu_{2\,CSA}$ $O_{4\,CSA}$ $Cu_{3\,CSA}$	$74.4°^{G}$	

					∠ $O_{1\,CSA}$ $Cu_{2\,CSA}$ $O_{4\,CSA}$	104.8 L	
					∠ $O_{1\,CSA}$ $Cu_{3\,CSA}$ $O_{4\,CSA}$	105.5 G	
					∠ $O_{1\,CSA}$ $Cu_{2\,CSA}$ Cu_{3CSA}	52.4° L	
					∠ $O_{1\,CSA}$ $Cu_{3\,CSA}$ Cu_{2CSA}	52.8° G	
					∠ $O_{4\,CSA}$ $Cu_{2\,CSA}$ Cu_{3CSA}		
					∠ $O_{4\,CSA}$ $Cu_{3\,CSA}$ Cu_{2CSA}		
		$Cu_{8\,CUS}$ $O_{1\,CSA}$ $Cu_{9\,CUS}$ $O_{4\,CSA}$	1.822^{L} 1.828^{G}	(b) 1.78	∠ $Cu_{2\,CSA}$ $O_{1\,CSA}$ $Cu_{8\,CUS}$ ∠ $Cu_{3\,CSA}$ $O_{1\,CSA}$ $Cu_{8\,CUS}$ ∠ $Cu_{2\,CSA}$ $O_{4\,CSA}$ $Cu_{9\,CUS}$ ∠ $Cu_{3\,CSA}$ $O_{4\,CSA}$ $Cu_{9\,CUS}$	141.1 L 138.7 G	
		$Cu_{6\,CSA}$ $O_{1\,CSA}$ $Cu_{5\,CSA}$ $O_{4\,CSA}$	1.956^{L} 1.966^{G}		∠ $Cu_{5\,CSA}$ $O_{4\,CSA}$ $Cu_{9\,CUS}$ ∠ $Cu_{6\,CSA}$ $O_{1\,CSA}$ $Cu_{8\,CUS}$	112.8 L 119.9 G	
		$Cu_{6\,CSA}$ $O_{7\,CUS}^{2}$ $Cu_{5\,CSA}$ $O_{7\,CUS}^{2}$	1.832^{L} 1.813^{G}		∠ $O_{4\,CSA}$ $Cu_{5\,CSA}$ $O_{7\,CUS}$ ∠ $O_{1\,CSA}$ $Cu_{6\,CSA}$ $O_{7\,CUS}$	147.7 L 147.8 G	
		$Cu_{2\,CSA}$ $Cu_{3\,CSA}$	2.470^{L} 2.488^{G}		∠ $Cu_{5\,CSA}$ $O_{7\,CUS}$ $Cu_{6\,CSA}$	85.8° L 87.2° G	
		$Cu_{5\,CSA}$ $Cu_{6\,CSA}$	2.493^{L} 2.5^{G}				
$(Cu_2O)_3$	C_{3v}	$Cu_{1\,CSA}$ $O_{4\,CUS}^{3}$ $Cu_{1\,CSA}$ $O_{5\,CUS}^{3}$ $Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$ $Cu_{2\,CSA}$ $O_{6\,CUS}^{3}$ $Cu_{3\,CSA}$ $O_{5\,CUS}^{3}$	1.832^{L} 1.912^{G}	(b) 1.91	∠ $Cu_{1\,CSA}$ $O_{4\,CSA}$ $Cu_{8\,CUS}$ ∠ $Cu_{2\,CSA}$ $O_{4\,CSA}$ $Cu_{8\,CUS}$ ∠ $Cu_{1\,CSA}$ $O_{5\,CSA}$ $Cu_{7\,CUS}$ ∠ $Cu_{3\,CSA}$ $O_{5\,CSA}$ $Cu_{7\,CUS}$ ∠ $Cu_{2\,CSA}$ $O_{6\,CSA}$ $Cu_{9\,CUS}$	136.1 L 101.2 G	(b) 109.6°

		$Cu_{3\,CSA}$ $O_{6\,CUS}^{3}$			∠ $Cu_{3\,CSA}$ $O_{6\,CSA}$ $Cu_{9\,CUS}$	
		$Cu_{7\,CUS}$ $O_{5\,CUS}^{3}$	1.762^{L}	(b) 1.77	∠ $Cu_{1\,CSA}$ $O_{4\,CSA}$ $Cu_{2\,CSA}$	$87.7°^{L}$
		$Cu_{8\,CUS}$ $O_{4\,CUS}^{3}$	1.811^{G}		∠ $Cu_{2\,CSA}$ $O_{6\,CSA}$ $Cu_{3\,CSA}$	$83.2°^{G}$
		$Cu_{9\,CUS}$ $O_{6\,CUS}^{3}$			∠ $Cu_{3\,CSA}$ $O_{5\,CSA}$ $Cu_{1\,CSA}$	
		$Cu_{1\,CSA}$ $Cu_{2\,CSA}$	2.539^{L}		∠ $O_{4\,CSA}$ $Cu_{1\,CSA}$ Cu_{2CSA}	$46°^{L}$
		$Cu_{2\,CSA}$ $Cu_{3\,CSA}$	2.539^{G}		∠ $O_{4\,CSA}$ $Cu_{2\,CSA}$ Cu_{1CSA}	$48.4°^{G}$
		$Cu_{1\,CSA}$ $Cu_{3\,CSA}$			∠ $O_{5\,CSA}$ $Cu_{1\,CSA}$ Cu_{3CSA}	
					∠ $O_{5\,CSA}$ $Cu_{3\,CSA}$ Cu_{1CSA}	
					∠ $O_{6\,CSA}$ $Cu_{2\,CSA}$ Cu_{3CSA}	
					∠ $O_{6\,CSA}$ $Cu_{3\,CSA}$ Cu_{2CSA}	
$(Cu_2O)_3$	C_s	$Cu_{2\,CSA}$ $O_{1\,CUS}^{2}$	1.776		∠ $Cu_{2\,CSA}$ $O_{1\,CUS}^{2}$ $Cu_{3\,CSA}$	114.2°
		$Cu_{3\,CSA}$ $O_{1\,CUS}^{2}$				
		$Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$	1.839		∠ $Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$ Cu_{6CUS}	108.3°
		$Cu_{3\,CSA}$ $O_{7\,CUS}^{3}$			∠ Cu_{3CSA} $O_{7\,CUS}^{3}$ Cu_{8CUS}	
		$Cu_{6\,CUS}$ $O_{4\,CUS}^{3}$	1.857		∠ $Cu_{2\,CSA}$ $O_{4\,CUS}^{3}$ $Cu_{5\,CUS}$	96.6°
		$Cu_{8\,CUS}$ $O_{7\,CUS}^{3}$			∠ $Cu_{3\,CSA}$ O_{7CUS}^{3} Cu_{9CUS}	
		$Cu_{5\,CUS}$ $O_{4\,CUS}^{3}$	1.872		∠ $Cu_{5\,CUS}$ $O_{4\,CUS}^{3}$ $Cu_{6\,CUS}$	86.2°
		$Cu_{9\,CUS}$ $O_{7\,CUS}^{3}$			∠ $Cu_{8\,CUS}$ $O_{7\,CUS}^{3}$ Cu_{9CUS}	

(a) is from reference 100.

(b) is from reference 101.

Table S5.2: Partial DOS (PDOS) data of Cu_2O clusters with increasing size at C_{2v} symmetry

Clusters	**Symmetry**	**Peaks**	**MOs. involved in Transition**		**MOs.**	**Contribution of AOs of Cu atom in forming MOs. (%)**			**Contribution of AOs of O atom in forming MOs.(%)**	
			Occupied	Virtual		s	p	d	s	p
$(Cu_2O)_1$	C_{2v}	1	5A1	5B1	5A1	30	2.1	30		34.08
					5B1	50	35.6			13.04
$(Cu_2O)_2$	C_{2v}	1	10B2	17A1	10B2	8		55.5	1.1	28.2
					17A1	61.6	25.5	6.4		21.01
$(Cu_2O)_3$	C_{2v}	1	14A1	13B2	14A1	26		25		44.41
					13B2	57.17	20.27	4.59		13.81

Table S5.3: Partial DOS (PDOS) data of Cu_2O clusters with fixed size at different symmetries

clusters	**Symmetry**	**peaks**	**MOs. involved in Transition**		**MOs.**	**Contribution of AOs of Cu atom in forming MOs. (%)**			**Contribution of AOs of O atom in forming MOs. (%)**	
			Occupied	Virtual		s	p	d	s	p
$(Cu_2O)_3$	C_s	2	20AAA	22AAA	20AAA	17.9	2.21	35.9		37
					22AAA	59.6	28			9.06
$(Cu_2O)_3$	C_{2v}	2	14A1	13B2	14A1	26		25		44.41
					13B2	57.17	20.27	4.59		13.81
$(Cu_2O)_3$	C_{3v}	2	95A	100A	95A	2.58		40.7		44.3
					100A	62.1	13.6			14.7

Table S5.4. Vibrational frequencies of clusters of different size and symmetry calculated using GGA as exchange and BLYP as correlation functional.

Clusters	**Symmetry**	**Frequencies (cm^{-1})**
$(Cu_2O)_1$	C_{2v}	ν_1= 99.011, ν_2 = 566.589, ν_3 = 594.664
$(Cu_2O)_2$	C_{2v}	ν_1 = 15.04, ν_2 = 49.45, ν_3 = 59.767, ν_4 = 74.66, ν_5 = 123.785, ν_6 = 150.66, ν_7 = 165.108, ν_8 =241.094, ν_9 =317.499, ν_{10} = 413.617, ν_{11} =525.733, ν_{12} =547.473
$(Cu_2O)_3$	C_{2v}	ν_1 = i13.422, ν_2 =17.442, ν_3 = 25.247, ν_4 = 45.538, ν_5 = 60.975, ν_6 = 97.623, ν_7 = 99.626, ν_8 = 103.112, ν_9 = 116.452, ν_{10} = 153.383, ν_{11} =195.809, ν_{12} = 197.193, ν_{13} = 199.533, ν_{14} = 206.058 ν_{15} =221.477, ν_{16} = 316.122, ν_{17} = 334.313, ν_{18} = 506.849, ν_{19} = 597.349, ν_{20} = 607.34, ν_{21} =612.904.
$(Cu_2O)_3$	C_{3v}	ν_1 = i17.692, ν_2 =10.035, ν_3 =11.067, ν_4 = 21.395, ν_5 = 27.751, ν_6 = 30.145, ν_7 = 103.919, ν_8 = 104.917, ν_9 = 133.134, ν_{10} = 147.902, ν_{11} = 148.521, ν_{12} = 200.889, ν_{13} = 342.961, ν_{14} = 344.991, ν_{15} = 408.415, ν_{16} = 449.01, ν_{17} = 484.134, ν_{18} = 486.374, ν_{19} = 563.883 ν_{20} = 566.764, ν_{21} = 584.341.
$(Cu_2O)_3$	C_s	ν_1 = i11.756, ν_2 = i1.781, ν_3 = 7.733, ν_4 = 12.833, ν_5 = 26.312, ν_6 = 34.469, ν_7 = 43.984 ν_8 = 86.646, ν_9 = 107.612, ν_{10} = 119.286, ν_{11} = 141.953, ν_{12} = 144.674, ν_{13} = 193.337, ν_{14} = 421.759, ν_{15} = 425.993, ν_{16} = 442.952, ν_{17} = 472.448, ν_{18} = 517.353, ν_{19} = 529.809, ν_{20} = 590.120, ν_{21} = 714.755.

Table S5.5: Partial DOS (PDOS) data of larger Cu_2O clusters with different size at fixed symmetries

clusters	**Symmetry**	**peaks**	**MOs. involved in Transition**		**MOs.**	**Contribution of AOs of Cu atom in forming MOs. (%)**			**Contribution of AOs of O atom in forming MOs.(%)**	
			Occupied	**Virtual**		***s***	***p***	***d***	***s***	***p***
$[Cu_{28}O_{15}]^{6+}$	$\boldsymbol{T_d}$	1	71T2	38A1	71T2			40		47
					38A1	74.86		15.45		10.75
$[Cu_{44}O_{15}]^{6+}$	$\boldsymbol{T_d}$	1	19A1	43T2	19A1	76.07		20.9		
					43T2	62.08		2.24		15.01

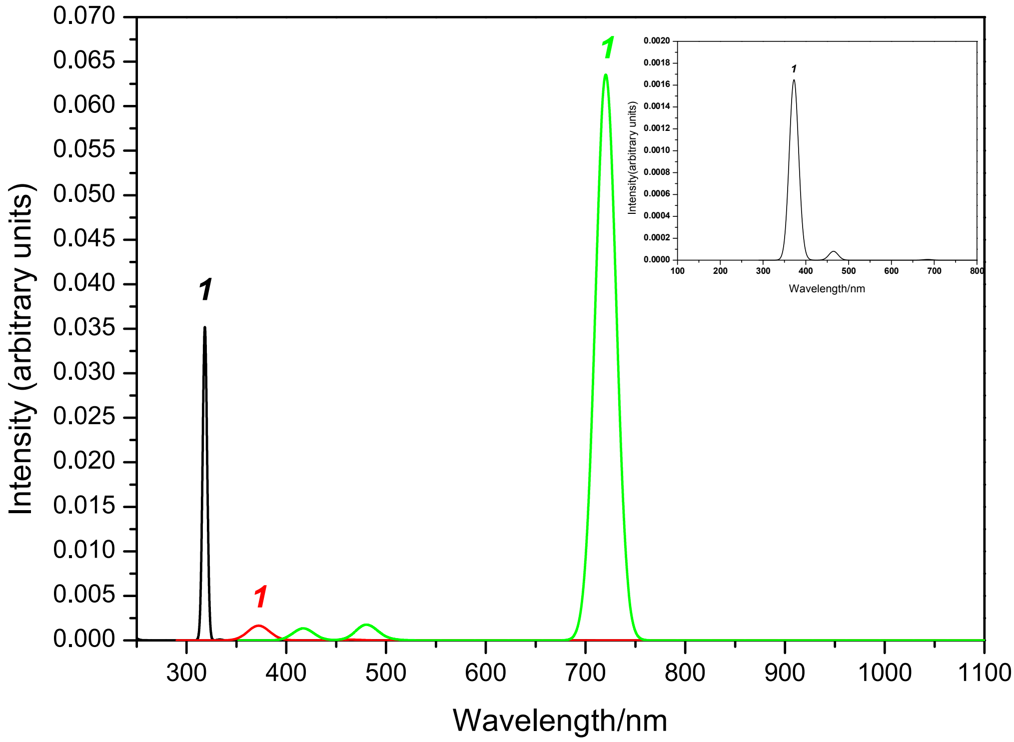

Figure S5.1: TDDFT valence excitation spectra (intensity vs wavelength) of $(Cu_2O)_1$ (black), $(Cu_2O)_2$ (red) and $(Cu_2O)_3$ (green) clusters having same symmetry (C_{2v}). Only the most intense discrete transitions are reported and labelled as 1. In the inset the intensity of peak ***1*** of $(Cu_2O)_2$ is displayed distinctly.

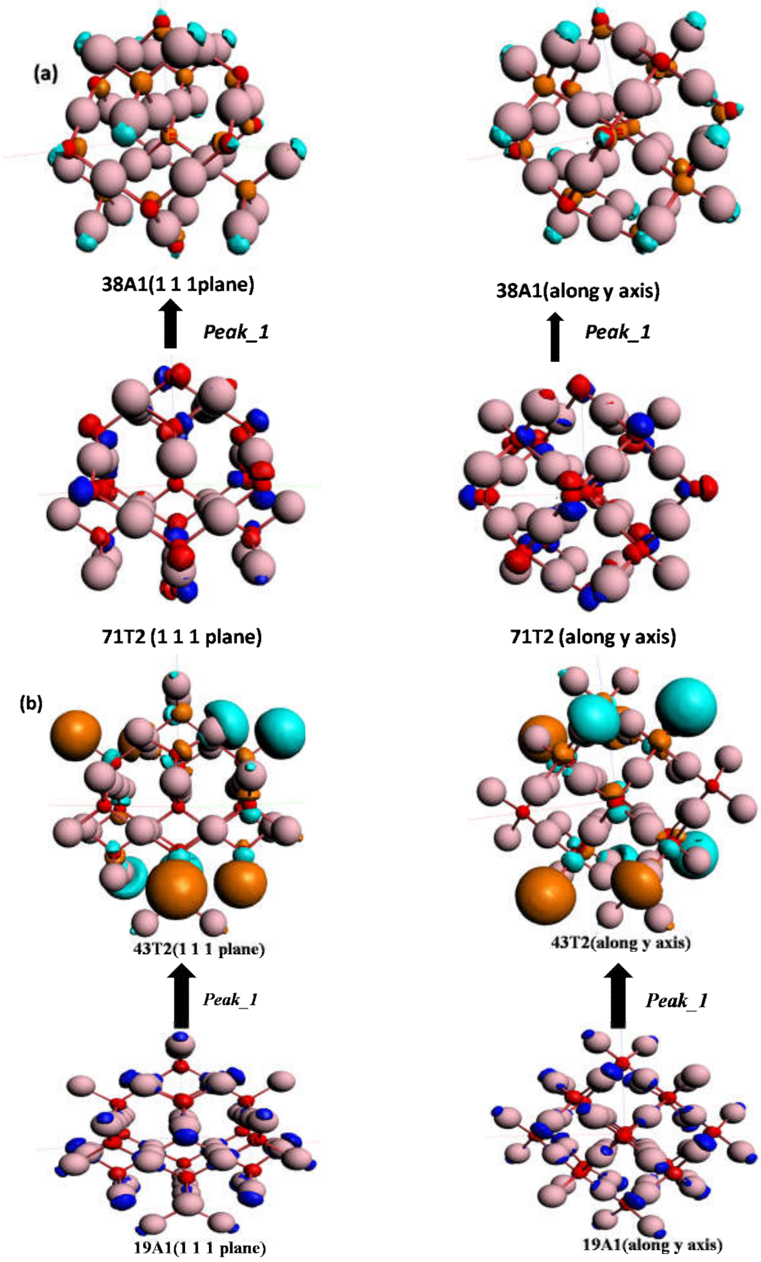

Figure S5.2: The representation of MOs participating in the electronic transitions to form the most intense peaks labelled as ***1*** (a) $[Cu_{28}O_{15}]^{6+}$ and (b) $[Cu_{44}O_{30}]^{6+}$ in T_d symmetry.

Chapter 6

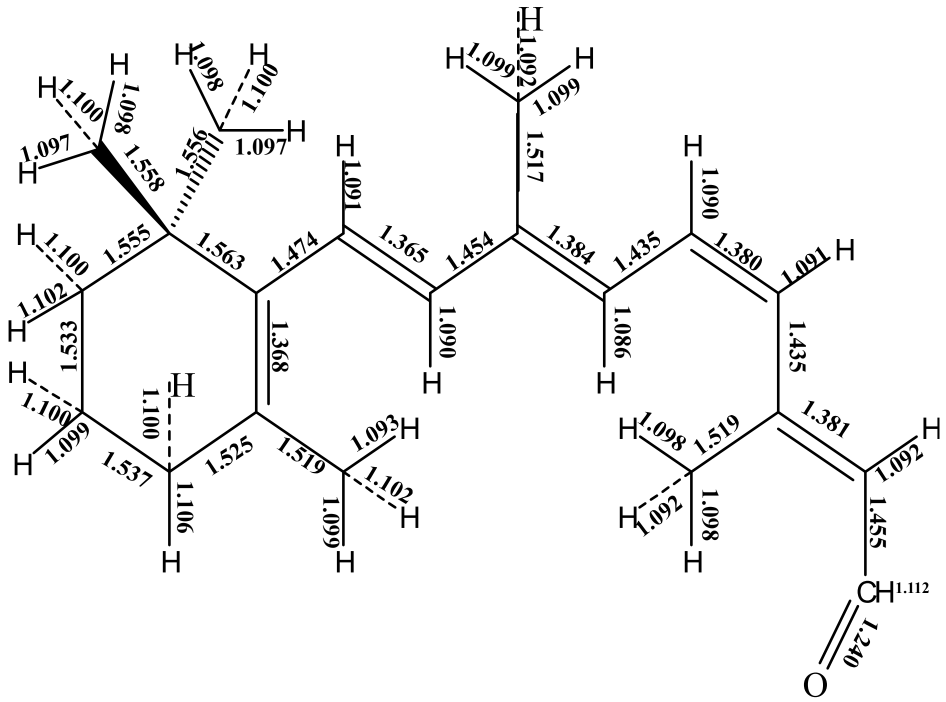

Figure S6.1 The optimised parameters (bond distances) of 11-cis retinal using GGA:BLYP functional.

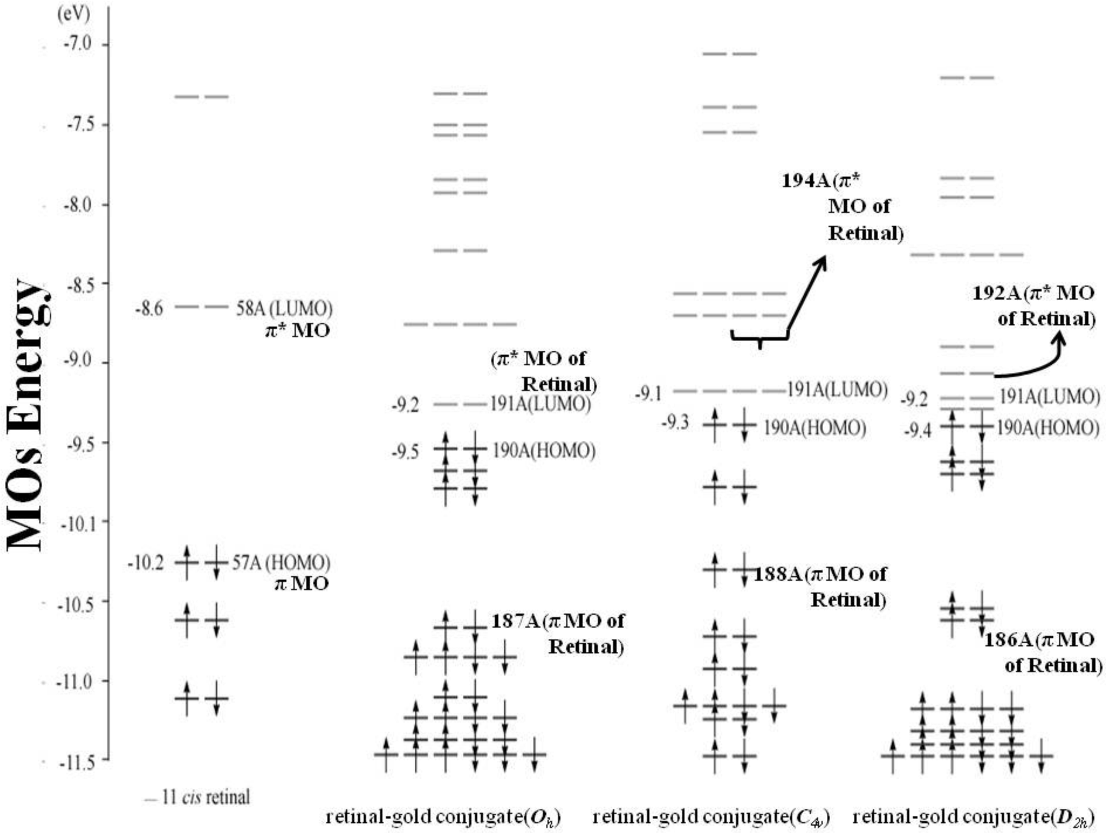

Figure S6.2 Energy level diagram of retinal and its gold conjugates

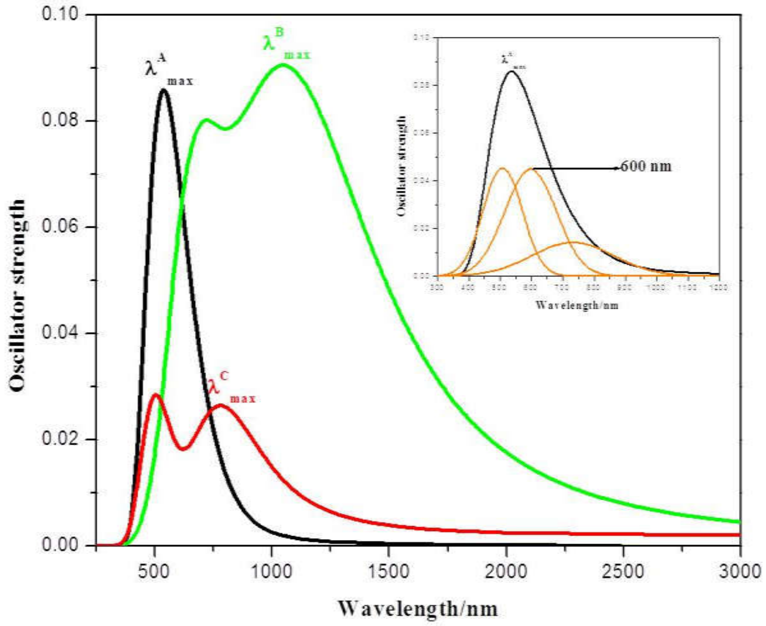

Figure S6.3 UV-visible excitation spectra with most intense excitations (λ_{max}) for retinal-cluster conjugate with symmetries O_h, D_{2h} and C_{4v} are shown in black ($\lambda^{A}{}_{max}$), green ($\lambda^{B}{}_{max}$), and red ($\lambda^{C}{}_{max}$) colors respectively. In the inset excitation peak of retinal gold (O_h) conjugate is deconvoluted further for better clarification.

Table S6.1 Vibrational frequencies of 11-*cis* retinal Au_{14} (O_h) conjugated system

$\tilde{\upsilon}_{1}$ i27.8.2 $\tilde{\upsilon}_{2}$ 19.4 $\tilde{\upsilon}_{3}$ i32.5 $\tilde{\upsilon}_{4}$ i13.2 $\tilde{\upsilon}$5 i5.5 $\tilde{\upsilon}_{6}$ 1.9 $\tilde{\upsilon}_{7}$ 6.3 $\tilde{\upsilon}_{8}$ 13.3 $\tilde{\upsilon}_{9}$ 15.02 $\tilde{\upsilon}_{10}$ 17.2 $\tilde{\upsilon}_{11}$ 18.2
$\tilde{\upsilon}_{12}$ 22.4 $\tilde{\upsilon}_{13}$ 28.3 $\tilde{\upsilon}_{14}$ 30.6 $\tilde{\upsilon}_{15}$ 32.2 $\tilde{\upsilon}_{16}$ 33.9 $\tilde{\upsilon}_{17}$ 39.7 $\tilde{\upsilon}_{18}$ 40.9 $\tilde{\upsilon}_{19}$ 42.2 $\tilde{\upsilon}_{20}$ 44.7 $\tilde{\upsilon}_{21}$46.8 $\tilde{\upsilon}_{22}$ 50.1 $\tilde{\upsilon}_{23}$
52.4 $\tilde{\upsilon}_{24}$ 53.9 $\tilde{\upsilon}_{25}$ 55.2 $\tilde{\upsilon}_{26}$ 58.8 $\tilde{\upsilon}_{27}$ 61.5 $\tilde{\upsilon}_{28}$ 62.7 $\tilde{\upsilon}_{29}$ 65.1 $\tilde{\upsilon}_{30}$ 67.9 $\tilde{\upsilon}_{31}$ 69.7 $\tilde{\upsilon}_{32}$ 75.5 $\tilde{\upsilon}_{33}$ 80.9
$\tilde{\upsilon}_{34}$ 81.4 $\tilde{\upsilon}_{35}$ 87.3 $\tilde{\upsilon}_{36}$ 88.4 $\tilde{\upsilon}_{37}$ 92.07 $\tilde{\upsilon}_{38}$ 96.8 $\tilde{\upsilon}_{39}$ 98.1 $\tilde{\upsilon}_{40}$ 101.5 $\tilde{\upsilon}_{41}$ 104.9 $\tilde{\upsilon}_{42}$ 107.9 $\tilde{\upsilon}_{43}$108.7
$\tilde{\upsilon}_{44}$ 114.5 $\tilde{\upsilon}_{45}$ 123.3 $\tilde{\upsilon}_{46}$ 124.9 $\tilde{\upsilon}_{47}$ 129.1 $\tilde{\upsilon}_{48}$ 131.2 $\tilde{\upsilon}_{49}$ 131.3 $\tilde{\upsilon}_{50}$ 139.6 $\tilde{\upsilon}_{51}$ 140.1 $\tilde{\upsilon}_{52}$ 148.2 $\tilde{\upsilon}_{53}$
170.4 $\tilde{\upsilon}_{54}$ 177.9 $\tilde{\upsilon}_{55}$ 197.3 $\tilde{\upsilon}_{56}$ 203.3 $\tilde{\upsilon}_{57}$ 218.1 $\tilde{\upsilon}_{58}$ 222.5 $\tilde{\upsilon}_{59}$ 238.7 $\tilde{\upsilon}_{60}$ 251.5 $\tilde{\upsilon}_{61}$ 262 $\tilde{\upsilon}_{62}$
264.8 $\tilde{\upsilon}_{63}$ 270.9 $\tilde{\upsilon}_{64}$ 291.2 $\tilde{\upsilon}_{65}$ 318.3 $\tilde{\upsilon}_{66}$ 327.9 $\tilde{\upsilon}_{67}$ 337.4 $\tilde{\upsilon}_{68}$ 342.4 $\tilde{\upsilon}_{69}$ 375.2 $\tilde{\upsilon}_{70}$ 383.8 $\tilde{\upsilon}_{71}$
404.1 $\tilde{\upsilon}_{72}$ 422 $\tilde{\upsilon}_{73}$ 447.9 $\tilde{\upsilon}_{74}$ 462.5 $\tilde{\upsilon}_{75}$ 485 $\tilde{\upsilon}_{76}$ 493.6 $\tilde{\upsilon}_{77}$ 509.3 $\tilde{\upsilon}_{78}$ 524.8 $\tilde{\upsilon}_{79}$ 557.8 $\tilde{\upsilon}_{80}$ 567.7
$\tilde{\upsilon}_{81}$ 580.4 $\tilde{\upsilon}_{82}$ 626.2 $\tilde{\upsilon}_{83}$ 687.3 $\tilde{\upsilon}_{84}$ 738.7 $\tilde{\upsilon}_{85}$ 764.6 $\tilde{\upsilon}_{86}$ 802.4 $\tilde{\upsilon}_{87}$ 805.8 $\tilde{\upsilon}_{88}$ 831.3 $\tilde{\upsilon}_{89}$ 834.6 $\tilde{\upsilon}_{90}$
858 $\tilde{\upsilon}_{91}$ 860 $\tilde{\upsilon}_{92}$ 880 $\tilde{\upsilon}_{93}$ 885 $\tilde{\upsilon}_{94}$ 901 $\tilde{\upsilon}_{95}$ 905.8 $\tilde{\upsilon}_{96}$ 909 $\tilde{\upsilon}_{97}$ 956.5 $\tilde{\upsilon}_{98}$ 959.5 $\tilde{\upsilon}_{99}$ 964.6 $\tilde{\upsilon}_{100}$
975.9 $\tilde{\upsilon}_{101}$ 979.8 $\tilde{\upsilon}_{102}$ 984.3 $\tilde{\upsilon}_{103}$ 987.7 $\tilde{\upsilon}_{104}$ 1001.7 $\tilde{\upsilon}_{105}$ 1008.7 $\tilde{\upsilon}_{106}$ 1027.7 $\tilde{\upsilon}_{107}$ 1030.9 $\tilde{\upsilon}_{108}$
1031.6 $\tilde{\upsilon}_{109}$ 1044.5 $\tilde{\upsilon}_{110}$ 1084.7 $\tilde{\upsilon}_{111}$ 1108.2 $\tilde{\upsilon}_{112}$ 1123.5 $\tilde{\upsilon}1_{13}$ 1147.5 $\tilde{\upsilon}_{114}$ 1156.4 $\tilde{\upsilon}_{115}$ 1166 $\tilde{\upsilon}_{116}$
1184.6 $\tilde{\upsilon}_{117}$ 1195.9 $\tilde{\upsilon}1_{18}$ 1203.3 $\tilde{\upsilon}_{119}$ 1221.3 $\tilde{\upsilon}_{120}$1242.1 $\tilde{\upsilon}_{121}$ 1263.8 $\tilde{\upsilon}_{122}$ 1270.4 $\tilde{\upsilon}_{123}$ 1298.4
$\tilde{\upsilon}_{124}$ 1311.4 $\tilde{\upsilon}_{125}$ 1331.1 $\tilde{\upsilon}_{126}$ 1332.7 $\tilde{\upsilon}_{127}$ 1334.9 $\tilde{\upsilon}_{128}$ 1349.2 $\tilde{\upsilon}_{129}$ 1352.8 $\tilde{\upsilon}_{130}$ 1361.3 $\tilde{\upsilon}_{131}$
1363.3 $\tilde{\upsilon}_{132}$ 1377.6 $\tilde{\upsilon}_{133}$ 1381.9 $\tilde{\upsilon}_{134}$ 1385.9 $\tilde{\upsilon}_{135}$ 1388.8 $\tilde{\upsilon}_{136}$ 1422.7 $\tilde{\upsilon}_{137}$ 1432.9 $\tilde{\upsilon}_{138}$ 1435.9
$\tilde{\upsilon}_{139}$ 1450 $\tilde{\upsilon}_{140}$ 1452.1 $\tilde{\upsilon}_{141}$ 1453.4 $\tilde{\upsilon}_{142}$ 1454.9 $\tilde{\upsilon}_{143}$ 1457.2 $\tilde{\upsilon}_{144}$ 1459.7 $\tilde{\upsilon}_{145}$ 1465.2 $\tilde{\upsilon}_{146}$ 1465.4
$\tilde{\upsilon}_{147}$ 1468.9 $\tilde{\upsilon}_{148}$ 1471 $\tilde{\upsilon}_{149}$ 1474.9 $\tilde{\upsilon}_{150}$ 1478.4 $\tilde{\upsilon}_{151}$ 1513.1 $\tilde{\upsilon}_{152}$ 1524.2 $\tilde{\upsilon}_{153}$ 1541 $\tilde{\upsilon}_{154}$ 1563
$\tilde{\upsilon}_{155}$ 1583 $\tilde{\upsilon}_{156}$ 2875.6 $\tilde{\upsilon}_{157}$ 2909.4 $\tilde{\upsilon}_{158}$ 2910 $\tilde{\upsilon}_{159}$ 2921.7 $\tilde{\upsilon}_{160}$ 2927.4 $\tilde{\upsilon}_{161}$ 2928.9 $\tilde{\upsilon}_{162}$ 2938.6
$\tilde{\upsilon}_{163}$ 2942.3 $\tilde{\upsilon}_{164}$ 2944.7 $\tilde{\upsilon}_{165}$ 2950 $\tilde{\upsilon}_{166}$ 2957.9 $\tilde{\upsilon}_{167}$ 2971.4 $\tilde{\upsilon}_{168}$ 2975.6 $\tilde{\upsilon}_{169}$ 2992.4 $\tilde{\upsilon}_{170}$ 2993.6
$\tilde{\upsilon}_{171}$ 2998 $\tilde{\upsilon}_{172}$ 3005.6 $\tilde{\upsilon}_{173}$ 3009.3 $\tilde{\upsilon}_{174}$ 3012.3 $\tilde{\upsilon}_{175}$ 3038.5 $\tilde{\upsilon}_{176}$ 3048.2 $\tilde{\upsilon}_{177}$ 3054.1 $\tilde{\upsilon}_{178}$
3059.5 $\tilde{\upsilon}_{179}$ 3069.2 $\tilde{\upsilon}_{180}$ 3070.2 $\tilde{\upsilon}_{181}$ 3076 $\tilde{\upsilon}_{182}$ 3077.1 $\tilde{\upsilon}_{183}$ 3114.2.

Table S6.2 Vibrational frequencies of 11-*cis* retinal Au$_{14}$ (D_{2h}) conjugated system

ῦ$_{1}$ i36.6 ῦ$_{2}$ i34.2 ῦ$_{3}$ i24.6 ῦ$_{4}$ i23.1 ῦ5 i21.9 ῦ$_{6}$ i17.7 ῦ$_{7}$ i12.1 ῦ$_{8}$ i8.5 ῦ$_{9}$ i2.9 ῦ$_{10}$ 2.1 ῦ$_{11}$ 7.4
ῦ$_{12}$ 11 ῦ$_{13}$ 14.3 ῦ$_{14}$ 17.5 ῦ$_{15}$ 18.1 ῦ$_{16}$ 18.9 ῦ$_{17}$ 23.1 ῦ$_{18}$ 28.2 ῦ$_{19}$ 31.8 ῦ$_{20}$ 34.1 ῦ$_{21}$39.3 ῦ$_{22}$ 41.1
ῦ$_{23}$ 44.5 ῦ$_{24}$ 47.6 ῦ$_{25}$ 51 ῦ$_{26}$ 54.1 ῦ$_{27}$ 57 ῦ$_{28}$ 58.1 ῦ$_{29}$ 60.5 ῦ$_{30}$ 61 ῦ$_{31}$ 63.7 ῦ$_{32}$ 64.3 ῦ$_{33}$ 66.8 ῦ$_{34}$ 68
ῦ$_{35}$ 70.1 ῦ$_{36}$ 73.5 ῦ$_{37}$ 74.9 ῦ$_{38}$ 75.4 ῦ$_{39}$ 79.2 ῦ$_{40}$ 85.7 ῦ$_{41}$ 86.5 ῦ$_{42}$ 87.3 ῦ$_{43}$ 91.2 ῦ$_{44}$ 102.3 ῦ$_{45}$ 108.2
ῦ$_{46}$ 114.3 ῦ$_{47}$ 115.5 ῦ$_{48}$ 120.9 ῦ$_{49}$ 124.5 ῦ$_{50}$ 129.7 ῦ$_{51}$ 132.5 ῦ$_{52}$ 143.1 ῦ$_{53}$ 167.8 ῦ$_{54}$ 180.1 ῦ$_{55}$
198.3 ῦ$_{56}$ 207.7 ῦ$_{57}$ 218.1 ῦ$_{58}$ 226 ῦ$_{59}$ 237.9 ῦ$_{60}$ 250.3 ῦ$_{61}$ 263.7 ῦ$_{62}$ 264.9 ῦ$_{63}$ 271.8 ῦ$_{64}$ 294.2 ῦ$_{65}$
318.4 ῦ$_{66}$ 323.5 ῦ$_{67}$ 339.5 ῦ$_{68}$ 342.4 ῦ$_{69}$ 372.8 ῦ$_{70}$ 384.8 ῦ$_{71}$ 404.1 ῦ$_{72}$ 420.2 ῦ$_{73}$ 449.9 ῦ$_{74}$ 463.7 ῦ$_{75}$
489.4 ῦ$_{76}$ 496 ῦ$_{77}$ 512.5 ῦ$_{78}$ 522.2 ῦ$_{79}$ 557.8 ῦ$_{80}$ 566.4 ῦ$_{81}$ 582 ῦ$_{82}$ 630.1 ῦ$_{83}$ 687.6 ῦ$_{84}$ 738.1 ῦ$_{85}$
765.4 ῦ$_{86}$ 804.3 ῦ$_{87}$ 807.2 ῦ$_{88}$ 830.4 ῦ$_{89}$ 832.6 ῦ$_{90}$ 858.6 ῦ$_{91}$ 861.4 ῦ$_{92}$ 881 ῦ$_{93}$ 887.7 ῦ$_{94}$ 901.5 ῦ$_{95}$
905.5 ῦ$_{96}$ 911.4 ῦ$_{97}$ 949.1 ῦ$_{98}$ 957 ῦ$_{99}$ 965.3 ῦ$_{100}$ 974.3 ῦ$_{101}$ 979.3 ῦ$_{102}$ 983.8 ῦ$_{103}$ 988.6 ῦ$_{104}$
1000.5 ῦ$_{105}$ 1007.8 ῦ$_{106}$ 1026.5 ῦ$_{107}$ 1030.7 ῦ$_{108}$ 1031 ῦ$_{109}$ 1043.9 ῦ$_{110}$ 1084.3 ῦ$_{111}$ 1108.2 ῦ$_{112}$
1124.1 ῦ1$_{13}$ 1148.1 ῦ$_{114}$ 1154.4 ῦ$_{115}$ 1170 ῦ$_{116}$ 1184.6 ῦ$_{117}$ 1196.7 ῦ1$_{18}$ 1202.6 ῦ$_{119}$ 1221.3
ῦ$_{120}$1242.1 ῦ$_{121}$ 1264.7 ῦ$_{122}$ 1270.6 ῦ$_{123}$ 1298.4 ῦ$_{124}$ 1319.9 ῦ$_{125}$ 1323.1 ῦ$_{126}$ 1333.3 ῦ$_{127}$ 1335.3
ῦ$_{128}$ 1348.1 ῦ$_{129}$ 1350.8 ῦ$_{130}$ 1357.3 ῦ$_{131}$ 1362.8 ῦ$_{132}$ 1377.5 ῦ$_{133}$ 1379.9 ῦ$_{134}$ 1384.7 ῦ$_{135}$
1388.8 ῦ$_{136}$ 1419.4 ῦ$_{137}$ 1429.8 ῦ$_{138}$ 1431.1 ῦ$_{139}$ 1450.3 ῦ$_{140}$ 1451.9 ῦ$_{141}$ 1453.7 ῦ$_{142}$ 1454.8
ῦ$_{143}$ 1456 ῦ$_{144}$ 1459.6 ῦ$_{145}$ 1465.8 ῦ$_{146}$ 1466.3 ῦ$_{147}$ 1468.9 ῦ$_{148}$ 1469.3 ῦ$_{149}$ 1472.7 ῦ$_{150}$ 1478.8
ῦ$_{151}$ 1507.2 ῦ$_{152}$ 1518.1 ῦ$_{153}$ 1532.6 ῦ$_{154}$ 1558 ῦ$_{155}$ 1580 ῦ$_{156}$ 2874.6 ῦ$_{157}$ 2911.4 ῦ$_{158}$ 2912.2
ῦ$_{159}$ 2923.2 ῦ$_{160}$ 2929 ῦ$_{161}$ 2930.1 ῦ$_{162}$ 2941.4 ῦ$_{163}$ 2942.8 ῦ$_{164}$ 2944.2 ῦ$_{165}$ 2960.1 ῦ$_{166}$ 2966.1
ῦ$_{167}$ 2977.2 ῦ$_{168}$ 2980.4 ῦ$_{169}$ 2995.1 ῦ$_{170}$ 2999 ῦ$_{171}$ 2999.2 ῦ$_{172}$ 3001.2 ῦ$_{173}$ 3012.4 ῦ$_{174}$ 3013.9
ῦ$_{175}$ 3028.5 ῦ$_{176}$ 3047.7 ῦ$_{177}$ 3062.9 ῦ$_{178}$ 3063.5 ῦ$_{179}$ 3067.3 ῦ$_{180}$ 3070.8 ῦ$_{181}$ 3075.7 ῦ$_{182}$
3095.7 ῦ$_{183}$ 3104.2.

Table S6.3 Vibrational frequencies of 11-*cis* retinal Au_{14} (C_{4v}) conjugated system

$\tilde{\upsilon}_{1}$ i29.2 $\tilde{\upsilon}_{2}$ i25.3 $\tilde{\upsilon}_{3}$ i20.7 $\tilde{\upsilon}_{4}$ i15.5 $\tilde{\upsilon}_{5}$ i11.9 $\tilde{\upsilon}_{6}$ i8.3 $\tilde{\upsilon}_{7}$ i5.9 $\tilde{\upsilon}_{8}$ i3.7 $\tilde{\upsilon}_{9}$ i2.3 $\tilde{\upsilon}_{10}$ 3.8 $\tilde{\upsilon}_{11}$ 8.5 $\tilde{\upsilon}_{12}$ 15.6 $\tilde{\upsilon}_{13}$ 16.8 $\tilde{\upsilon}_{14}$ 22.8 $\tilde{\upsilon}_{15}$ 25.1 $\tilde{\upsilon}_{16}$ 27.5 $\tilde{\upsilon}_{17}$ 28.8 $\tilde{\upsilon}_{18}$ 30.4 $\tilde{\upsilon}_{19}$ 33.4 $\tilde{\upsilon}_{20}$ 35.2 $\tilde{\upsilon}_{21}$ 41.6 $\tilde{\upsilon}_{22}$ 42.6 $\tilde{\upsilon}_{23}$ 44.9 $\tilde{\upsilon}_{24}$ 46.1 $\tilde{\upsilon}_{25}$ 46.8 $\tilde{\upsilon}_{26}$ 48.4 $\tilde{\upsilon}_{27}$ 49.9 $\tilde{\upsilon}_{28}$ 52.6 $\tilde{\upsilon}_{29}$ 55.4 $\tilde{\upsilon}_{30}$ 57.1 $\tilde{\upsilon}_{31}$ 60.8 $\tilde{\upsilon}_{32}$ 63 $\tilde{\upsilon}_{33}$ 72.7 $\tilde{\upsilon}_{34}$ 74.5 $\tilde{\upsilon}_{35}$ 83.9 $\tilde{\upsilon}_{36}$ 85.8 $\tilde{\upsilon}_{37}$ 95.9 $\tilde{\upsilon}_{38}$ 99.4 $\tilde{\upsilon}_{39}$ 99.9 $\tilde{\upsilon}_{40}$ 102.6 $\tilde{\upsilon}_{41}$ 105.7 $\tilde{\upsilon}_{42}$ 106.7 $\tilde{\upsilon}_{43}$ 107.2 $\tilde{\upsilon}_{44}$ 117.2 $\tilde{\upsilon}_{45}$ 119.9 $\tilde{\upsilon}_{46}$ 123.1 $\tilde{\upsilon}_{47}$ 134.8 $\tilde{\upsilon}_{48}$ 140.2 $\tilde{\upsilon}_{49}$ 141.4 $\tilde{\upsilon}_{50}$ 144.6 $\tilde{\upsilon}_{51}$ 153.7 $\tilde{\upsilon}_{52}$ 154.4 $\tilde{\upsilon}_{53}$ 160.2 $\tilde{\upsilon}_{54}$ 170.8 $\tilde{\upsilon}_{55}$ 190.4 $\tilde{\upsilon}_{56}$ 214 $\tilde{\upsilon}_{57}$ 221.6 $\tilde{\upsilon}_{58}$ 236.4 $\tilde{\upsilon}_{59}$ 250.1 $\tilde{\upsilon}_{60}$ 252.3 $\tilde{\upsilon}_{61}$ 262.9 $\tilde{\upsilon}_{62}$ 266.4 $\tilde{\upsilon}_{63}$ 287.3 $\tilde{\upsilon}_{64}$ 309.7 $\tilde{\upsilon}_{65}$ 315.9 $\tilde{\upsilon}_{66}$ 333.7 $\tilde{\upsilon}_{67}$ 341.7 $\tilde{\upsilon}_{68}$ 374.8 $\tilde{\upsilon}_{69}$ 384 $\tilde{\upsilon}_{70}$ 402.9 $\tilde{\upsilon}_{71}$ 418.3 $\tilde{\upsilon}_{72}$ 440.4 $\tilde{\upsilon}_{73}$ 461 $\tilde{\upsilon}_{74}$ 470 $\tilde{\upsilon}_{75}$ 487 $\tilde{\upsilon}_{76}$ 500.8 $\tilde{\upsilon}_{77}$ 522.1 $\tilde{\upsilon}_{78}$ 557.2 $\tilde{\upsilon}_{79}$ 565.4 $\tilde{\upsilon}_{80}$ 573.8 $\tilde{\upsilon}_{81}$ 625.2 $\tilde{\upsilon}_{82}$ 686.8 $\tilde{\upsilon}_{83}$ 738 $\tilde{\upsilon}_{84}$ 764 $\tilde{\upsilon}_{85}$ 792.7 $\tilde{\upsilon}_{86}$ 801.8 $\tilde{\upsilon}_{87}$ 829 $\tilde{\upsilon}_{88}$ 834.3 $\tilde{\upsilon}_{89}$ 853.8 $\tilde{\upsilon}_{90}$ 859.6 $\tilde{\upsilon}_{91}$ 878.3 $\tilde{\upsilon}_{92}$ 881 $\tilde{\upsilon}_{93}$ 900.4 $\tilde{\upsilon}_{94}$ 903 $\tilde{\upsilon}_{95}$ 907.9 $\tilde{\upsilon}_{96}$ 956.5 $\tilde{\upsilon}_{97}$ 962.1 $\tilde{\upsilon}_{98}$ 965.8 $\tilde{\upsilon}_{99}$ 974.1 $\tilde{\upsilon}_{100}$ 977.9 $\tilde{\upsilon}_{101}$ 983.1 $\tilde{\upsilon}_{102}$ 987.3 $\tilde{\upsilon}_{103}$ 1001.2 $\tilde{\upsilon}_{104}$ 1008.3 $\tilde{\upsilon}_{105}$ 1028.3 $\tilde{\upsilon}_{106}$ 1031.7 $\tilde{\upsilon}_{107}$ 1034.3 $\tilde{\upsilon}_{108}$ 1043.8 $\tilde{\upsilon}_{109}$ 1074.4 $\tilde{\upsilon}_{110}$ 1105 $\tilde{\upsilon}_{111}$ 1115.3 $\tilde{\upsilon}_{112}$ 1128.4 $\tilde{\upsilon}_{113}$ 1147.1 $\tilde{\upsilon}_{114}$ 1156.1 $\tilde{\upsilon}_{115}$ 1183.9 $\tilde{\upsilon}_{116}$ 1195.5 $\tilde{\upsilon}_{117}$ 1197.5 $\tilde{\upsilon}_{118}$ 1212.7 $\tilde{\upsilon}_{119}$ 1240.6 $\tilde{\upsilon}_{120}$ 1269.9 $\tilde{\upsilon}_{121}$ 1270.2 $\tilde{\upsilon}_{122}$ 1291.7 $\tilde{\upsilon}_{123}$ 1313.5 $\tilde{\upsilon}_{124}$ 1331.9 $\tilde{\upsilon}_{125}$ 1333.4 $\tilde{\upsilon}_{126}$ 1334 $\tilde{\upsilon}_{127}$ 1344.5 $\tilde{\upsilon}_{128}$ 1348.3 $\tilde{\upsilon}_{129}$ 1360.9 $\tilde{\upsilon}_{130}$ 1369.3 $\tilde{\upsilon}_{131}$ 1377.7 $\tilde{\upsilon}_{132}$ 1383.6 $\tilde{\upsilon}_{133}$ 1384.6 $\tilde{\upsilon}_{134}$ 1386.2 $\tilde{\upsilon}_{135}$ 1430 $\tilde{\upsilon}_{136}$ 1436 $\tilde{\upsilon}_{137}$ 1447.3 $\tilde{\upsilon}_{138}$ 1449.5 $\tilde{\upsilon}_{139}$ 1453.5 $\tilde{\upsilon}_{140}$ 1454.4 $\tilde{\upsilon}_{141}$ 1455.3 $\tilde{\upsilon}_{142}$ 1459.2 $\tilde{\upsilon}_{143}$ 1460.5 $\tilde{\upsilon}_{144}$ 1463.9.6 $\tilde{\upsilon}_{145}$ 1465.1 $\tilde{\upsilon}_{146}$ 1468 $\tilde{\upsilon}_{147}$ 1470 $\tilde{\upsilon}_{148}$ 1478 $\tilde{\upsilon}_{149}$ 1501.6 $\tilde{\upsilon}_{150}$ 1520.6 $\tilde{\upsilon}_{151}$ 1544.9 $\tilde{\upsilon}_{152}$ 1559.9 $\tilde{\upsilon}_{153}$ 1584.7 $\tilde{\upsilon}_{154}$ 1594.2 $\tilde{\upsilon}_{155}$ 2820.2 $\tilde{\upsilon}_{156}$ 2875.8 $\tilde{\upsilon}_{157}$ 2908.1 $\tilde{\upsilon}_{158}$ 2910.1 $\tilde{\upsilon}_{159}$ 2921.9 $\tilde{\upsilon}_{160}$ 2925.9 $\tilde{\upsilon}_{161}$ 2928.7 $\tilde{\upsilon}_{162}$ 2935 $\tilde{\upsilon}_{163}$ 2939.9 $\tilde{\upsilon}_{164}$ 2940.3 $\tilde{\upsilon}_{165}$ 2956.8 $\tilde{\upsilon}_{166}$ 2965.2 $\tilde{\upsilon}_{167}$ 2973.1 $\tilde{\upsilon}_{168}$ 2987.4 $\tilde{\upsilon}_{169}$ 2994 $\tilde{\upsilon}_{170}$ 2998.2 $\tilde{\upsilon}_{171}$ 2999 $\tilde{\upsilon}_{172}$ 3010.9 $\tilde{\upsilon}_{173}$ 3013.6 $\tilde{\upsilon}_{174}$ 3036.8 $\tilde{\upsilon}_{175}$ 3044.3 $\tilde{\upsilon}_{176}$ 3053.4 $\tilde{\upsilon}_{177}$ 3059 $\tilde{\upsilon}_{178}$ 3059.7 $\tilde{\upsilon}_{179}$ 3063.6 $\tilde{\upsilon}_{180}$ 3067.7 $\tilde{\upsilon}_{181}$ 3075 $\tilde{\upsilon}_{182}$ 3095.7 $\tilde{\upsilon}_{183}$ 3098.4.

Table S6.4 Vibrational frequencies of all *trans* retinal Au_{14} (O_h) conjugated system

$\tilde{\upsilon}_{1}$ i18.2 $\tilde{\upsilon}_{2}$ i11.6 $\tilde{\upsilon}_{3}$ i8.9 $\tilde{\upsilon}_{4}$ i3.1 $\tilde{\upsilon}$5 3.7 $\tilde{\upsilon}_{6}$ 9.4 $\tilde{\upsilon}_{7}$ 12.2 $\tilde{\upsilon}_{8}$ 14.3 $\tilde{\upsilon}_{9}$ 14.7 $\tilde{\upsilon}_{10}$ 17 $\tilde{\upsilon}_{11}$ 20.5 $\tilde{\upsilon}_{12}$ 26 $\tilde{\upsilon}_{13}$ 28.6 $\tilde{\upsilon}_{14}$ 29 $\tilde{\upsilon}_{15}$ 32.2 $\tilde{\upsilon}_{16}$ 37.2 $\tilde{\upsilon}_{17}$ 40.1 $\tilde{\upsilon}_{18}$ 40.3 $\tilde{\upsilon}_{19}$ 45.5 $\tilde{\upsilon}_{20}$ 46.4 $\tilde{\upsilon}_{21}$ 48.7 $\tilde{\upsilon}_{22}$ 50.7 $\tilde{\upsilon}_{23}$ 51.3 $\tilde{\upsilon}_{24}$ 53 $\tilde{\upsilon}_{25}$ 56.2 $\tilde{\upsilon}_{26}$ 58.5 $\tilde{\upsilon}_{27}$ 59.7 $\tilde{\upsilon}_{28}$ 61.3 $\tilde{\upsilon}_{29}$ 66.2 $\tilde{\upsilon}_{30}$ 67.6 $\tilde{\upsilon}_{31}$ 68 $\tilde{\upsilon}_{32}$ 76 $\tilde{\upsilon}_{33}$ 80.8 $\tilde{\upsilon}_{34}$ 88 $\tilde{\upsilon}_{35}$ 90.7 $\tilde{\upsilon}_{36}$ 97.2 $\tilde{\upsilon}_{37}$ 98.5 $\tilde{\upsilon}_{38}$ 100.3 $\tilde{\upsilon}_{39}$ 100.4 $\tilde{\upsilon}_{40}$ 105 $\tilde{\upsilon}_{41}$ 106.7 $\tilde{\upsilon}_{42}$ 108.3 $\tilde{\upsilon}_{43}$ 111.4 $\tilde{\upsilon}_{44}$ 117.3 $\tilde{\upsilon}_{45}$ 127.8 $\tilde{\upsilon}_{46}$ 129.4 $\tilde{\upsilon}_{47}$ 131.1 $\tilde{\upsilon}_{48}$ 133.1 $\tilde{\upsilon}_{49}$ 133.8 $\tilde{\upsilon}_{50}$ 134.2 $\tilde{\upsilon}_{51}$ 137.6 $\tilde{\upsilon}_{52}$ 146.6 $\tilde{\upsilon}_{53}$ 155.4 $\tilde{\upsilon}_{54}$ 161.6 $\tilde{\upsilon}_{55}$ 175 $\tilde{\upsilon}_{56}$ 199.1 $\tilde{\upsilon}_{57}$ 221.4 $\tilde{\upsilon}_{58}$ 227.3 $\tilde{\upsilon}_{59}$ 247.8 $\tilde{\upsilon}_{60}$ 250.9 $\tilde{\upsilon}_{61}$ 260.9 $\tilde{\upsilon}_{62}$ 266.1 $\tilde{\upsilon}_{63}$ 289.2 $\tilde{\upsilon}_{64}$ 299.7 $\tilde{\upsilon}_{65}$ 311.7 $\tilde{\upsilon}_{66}$ 318 $\tilde{\upsilon}_{67}$ 330.7 351.2 $\tilde{\upsilon}_{68}$ 356.3 $\tilde{\upsilon}_{69}$ 371.8 $\tilde{\upsilon}_{70}$ 406.2 $\tilde{\upsilon}_{71}$ 414.6 $\tilde{\upsilon}_{72}$ 425.6 $\tilde{\upsilon}_{73}$ 464 $\tilde{\upsilon}_{74}$ 482.7 $\tilde{\upsilon}_{75}$ 491.2 $\tilde{\upsilon}_{76}$ 505.5 $\tilde{\upsilon}_{77}$ 526.8 $\tilde{\upsilon}_{78}$ 548.8 $\tilde{\upsilon}_{79}$ 557.4 $\tilde{\upsilon}_{80}$ 593.9 $\tilde{\upsilon}_{81}$ 625.8 $\tilde{\upsilon}_{82}$ 648.2 $\tilde{\upsilon}_{83}$ 714.9 $\tilde{\upsilon}_{84}$ 764.4 $\tilde{\upsilon}_{85}$ 807.9 $\tilde{\upsilon}_{86}$ 833.4 $\tilde{\upsilon}_{87}$ 837.2 $\tilde{\upsilon}_{88}$ 844.1 $\tilde{\upsilon}_{89}$ 859 $\tilde{\upsilon}_{90}$ 863.5 $\tilde{\upsilon}_{91}$ 879.9 $\tilde{\upsilon}_{92}$ 894.8 $\tilde{\upsilon}_{93}$ 900.3 $\tilde{\upsilon}_{94}$ 902.9 $\tilde{\upsilon}_{95}$ 908 $\tilde{\upsilon}_{96}$ 941.1 $\tilde{\upsilon}_{97}$ 957 $\tilde{\upsilon}_{98}$ 963.9 $\tilde{\upsilon}_{99}$ 976.1 $\tilde{\upsilon}_{100}$ 983.5 $\tilde{\upsilon}_{101}$ 986.2 $\tilde{\upsilon}_{102}$ 998.9 $\tilde{\upsilon}_{103}$ 1004.1 $\tilde{\upsilon}_{104}$ 1019.3 $\tilde{\upsilon}_{105}$ 1027.8 $\tilde{\upsilon}_{106}$ 1031.4 $\tilde{\upsilon}_{107}$ 1031.8 $\tilde{\upsilon}_{108}$ 1044.1 $\tilde{\upsilon}_{109}$ 1104.1 $\tilde{\upsilon}_{110}$ 1118.1 $\tilde{\upsilon}_{111}$ 1141.8 $\tilde{\upsilon}_{112}$ 1148.6 $\tilde{\upsilon}_{113}$ 1155.6 $\tilde{\upsilon}_{114}$ 1177.3 $\tilde{\upsilon}_{115}$ 1184.6 $\tilde{\upsilon}_{116}$ 1193.8 $\tilde{\upsilon}_{117}$ 1197.1 $\tilde{\upsilon}_{118}$ 1223.5 $\tilde{\upsilon}_{119}$ 1242.2 $\tilde{\upsilon}_{120}$ 1266.2 $\tilde{\upsilon}_{121}$ 1270.6 $\tilde{\upsilon}_{122}$ 1288.6 $\tilde{\upsilon}_{123}$ 1308.7 $\tilde{\upsilon}_{124}$ 1313 $\tilde{\upsilon}_{125}$ 1326.3 $\tilde{\upsilon}_{126}$ 1332.4 $\tilde{\upsilon}_{127}$ 1335.2 $\tilde{\upsilon}_{128}$ 1348.2 $\tilde{\upsilon}_{129}$ 1353.2 $\tilde{\upsilon}_{130}$ 1362.4 $\tilde{\upsilon}_{131}$ 1368.2 $\tilde{\upsilon}_{132}$ 1378.4 $\tilde{\upsilon}_{133}$ 1384 $\tilde{\upsilon}_{134}$ 1385.3 $\tilde{\upsilon}_{135}$ 1387.3 $\tilde{\upsilon}_{136}$ 1436.4 $\tilde{\upsilon}_{137}$ 1445.3 $\tilde{\upsilon}_{138}$ 1449.5 $\tilde{\upsilon}_{139}$ 1452.2 $\tilde{\upsilon}_{140}$ 1453.2 $\tilde{\upsilon}_{141}$ 1455 $\tilde{\upsilon}_{142}$ 1458 $\tilde{\upsilon}_{143}$ 1459.6 $\tilde{\upsilon}_{144}$ 1464.3 $\tilde{\upsilon}_{145}$ 1464.6 $\tilde{\upsilon}_{146}$ 1468.8 $\tilde{\upsilon}_{147}$ 1471.6 $\tilde{\upsilon}_{148}$ 1477.8 $\tilde{\upsilon}_{149}$ 1480.9 $\tilde{\upsilon}_{150}$ 1505.8 $\tilde{\upsilon}_{151}$ 1531.8 $\tilde{\upsilon}_{152}$ 1544.8 $\tilde{\upsilon}_{153}$ 1569.2 $\tilde{\upsilon}_{154}$ 1586.9 $\tilde{\upsilon}_{155}$ 2874.7 $\tilde{\upsilon}_{156}$ 2912.9 $\tilde{\upsilon}_{157}$ 2913 $\tilde{\upsilon}_{158}$ 2922.9 $\tilde{\upsilon}_{159}$ 2928.7 $\tilde{\upsilon}_{160}$ 2930.1 $\tilde{\upsilon}_{161}$ 2931 $\tilde{\upsilon}_{162}$ 2936 $\tilde{\upsilon}_{163}$ 2941.9 $\tilde{\upsilon}_{164}$ 2944.5 $\tilde{\upsilon}_{165}$ 2960.3 $\tilde{\upsilon}_{166}$ 2974.9 $\tilde{\upsilon}_{167}$ 2976.5 $\tilde{\upsilon}_{168}$ 2990.1 $\tilde{\upsilon}_{169}$ 2993.7 $\tilde{\upsilon}_{170}$ 2997.7 $\tilde{\upsilon}_{171}$ 2998.7 $\tilde{\upsilon}_{172}$ 3010.3 $\tilde{\upsilon}_{173}$ 3015.1 $\tilde{\upsilon}_{174}$ 3037.4 $\tilde{\upsilon}_{175}$ 3040.1 $\tilde{\upsilon}_{176}$ 3047.9 $\tilde{\upsilon}_{177}$ 3053.2 $\tilde{\upsilon}_{178}$ 3054.1 $\tilde{\upsilon}_{179}$ 3056.6 $\tilde{\upsilon}_{180}$ 3066.8 $\tilde{\upsilon}_{181}$ 3070 $\tilde{\upsilon}_{182}$ 3080.8 $\tilde{\upsilon}_{183}$ 3088.8.

Table S6.5 Vibrational frequencies of all *trans* retinal Au_{14} (D_{2h}) conjugated system

$\tilde{\upsilon}_{1}$ i34.9 $\tilde{\upsilon}_{2}$ i26.5 $\tilde{\upsilon}_{3}$ i23.5 $\tilde{\upsilon}_{4}$ i19.9 $\tilde{\upsilon}$5 i8.4 $\tilde{\upsilon}_{6}$ i6.6 $\tilde{\upsilon}_{7}$ i3.6 $\tilde{\upsilon}_{8}$ 7.2 $\tilde{\upsilon}_{9}$ 7.9 $\tilde{\upsilon}_{10}$ 9.9 $\tilde{\upsilon}_{11}$ 11.2 $\tilde{\upsilon}_{12}$ 13.8 $\tilde{\upsilon}_{13}$ 14.6 $\tilde{\upsilon}_{14}$ 16.3 $\tilde{\upsilon}_{15}$ 20.8 $\tilde{\upsilon}_{16}$ 23.5 $\tilde{\upsilon}_{17}$ 28.7 $\tilde{\upsilon}_{18}$ 30.2 $\tilde{\upsilon}_{19}$ 36.3 $\tilde{\upsilon}_{20}$ 37.4 $\tilde{\upsilon}_{21}$ 44.5 $\tilde{\upsilon}_{22}$ 46.8 $\tilde{\upsilon}_{23}$ 51.8 $\tilde{\upsilon}_{24}$ 55.3 $\tilde{\upsilon}_{25}$ 57.4 $\tilde{\upsilon}_{26}$ 61.5 $\tilde{\upsilon}_{27}$ 63.6 $\tilde{\upsilon}_{28}$ 64.6 $\tilde{\upsilon}_{29}$ 66.1 $\tilde{\upsilon}_{30}$ 68.2 $\tilde{\upsilon}_{31}$ 70.5 $\tilde{\upsilon}_{32}$ 72.3 $\tilde{\upsilon}_{33}$ 74.7 $\tilde{\upsilon}_{34}$ 76.1 $\tilde{\upsilon}_{35}$ 79.3 $\tilde{\upsilon}_{36}$ 80.9 $\tilde{\upsilon}_{37}$ 81.2 $\tilde{\upsilon}_{38}$ 81.8 $\tilde{\upsilon}_{39}$ 83.4 $\tilde{\upsilon}_{40}$ 87.2 $\tilde{\upsilon}_{41}$ 94 $\tilde{\upsilon}_{42}$ 95.3 $\tilde{\upsilon}_{43}$ 102.9 $\tilde{\upsilon}_{44}$ 107.6 $\tilde{\upsilon}_{45}$ 116 $\tilde{\upsilon}_{46}$ 124.1 $\tilde{\upsilon}_{47}$ 128.6 $\tilde{\upsilon}_{48}$ 131.4 $\tilde{\upsilon}_{49}$ 134.7 $\tilde{\upsilon}_{50}$ 136.5 $\tilde{\upsilon}_{51}$ 138.9 $\tilde{\upsilon}_{52}$ 162.9 $\tilde{\upsilon}_{53}$ 168.8 $\tilde{\upsilon}_{54}$ 180.8 $\tilde{\upsilon}_{55}$ 191.4 $\tilde{\upsilon}_{56}$ 219.7 $\tilde{\upsilon}_{57}$ 229.7 $\tilde{\upsilon}_{58}$ 247 $\tilde{\upsilon}_{59}$ 261 $\tilde{\upsilon}_{60}$ 265.4 $\tilde{\upsilon}_{61}$ 270 $\tilde{\upsilon}_{62}$ 278.9 $\tilde{\upsilon}_{63}$ 300 $\tilde{\upsilon}_{64}$ 314.1 $\tilde{\upsilon}_{65}$ 328.9 $\tilde{\upsilon}_{66}$ 336.1 $\tilde{\upsilon}_{67}$ 350.6 $\tilde{\upsilon}_{68}$ 363.6 $\tilde{\upsilon}_{69}$ 381.4 $\tilde{\upsilon}_{70}$ 414.3 $\tilde{\upsilon}_{71}$ 423.54 $\tilde{\upsilon}_{72}$ 433 $\tilde{\upsilon}_{73}$ 474.4 $\tilde{\upsilon}_{74}$ 493.9 $\tilde{\upsilon}_{75}$ 502.4 $\tilde{\upsilon}_{76}$ 512.4 $\tilde{\upsilon}_{77}$ 534.4 $\tilde{\upsilon}_{78}$ 546.8 $\tilde{\upsilon}_{79}$ 564.6 $\tilde{\upsilon}_{80}$ 605.7 $\tilde{\upsilon}_{81}$ 633.2 $\tilde{\upsilon}_{82}$ 659.5 $\tilde{\upsilon}_{83}$ 724.3 $\tilde{\upsilon}_{84}$ 766.8 $\tilde{\upsilon}_{85}$ 805.6 $\tilde{\upsilon}_{86}$ 835.6 $\tilde{\upsilon}_{87}$ 845.9 $\tilde{\upsilon}_{88}$ 851.6 $\tilde{\upsilon}_{89}$ 869.8 $\tilde{\upsilon}_{90}$ 874.4 $\tilde{\upsilon}_{91}$ 891.3 $\tilde{\upsilon}_{92}$ 905.4 $\tilde{\upsilon}_{93}$ 909.3 $\tilde{\upsilon}_{94}$ 909.8 $\tilde{\upsilon}_{95}$ 917.6 $\tilde{\upsilon}_{96}$ 936.6 $\tilde{\upsilon}_{97}$ 957.7 $\tilde{\upsilon}_{98}$ 976.6 $\tilde{\upsilon}_{99}$ 982.5 $\tilde{\upsilon}_{100}$ 994.5 $\tilde{\upsilon}_{101}$ 1003.7 $\tilde{\upsilon}_{102}$ 1018.1 $\tilde{\upsilon}_{103}$ 1028.5 $\tilde{\upsilon}_{104}$ 1044.2 $\tilde{\upsilon}_{105}$ 1050.8 $\tilde{\upsilon}_{106}$ 1062 $\tilde{\upsilon}_{107}$ 1063.5 $\tilde{\upsilon}_{108}$ 1067.5 $\tilde{\upsilon}_{109}$ 1118.6 $\tilde{\upsilon}_{110}$ 1138.1 $\tilde{\upsilon}_{111}$ 1150.9 $\tilde{\upsilon}_{112}$ 1161.9 $\tilde{\upsilon}_{113}$ 1175.1 $\tilde{\upsilon}_{114}$ 1195.8 $\tilde{\upsilon}_{115}$ 1201.5 $\tilde{\upsilon}_{116}$ 1209.4 $\tilde{\upsilon}_{117}$ 1220.6 $\tilde{\upsilon}_{118}$ 1235.2 $\tilde{\upsilon}_{119}$ 1262.5 $\tilde{\upsilon}_{120}$ 1281 $\tilde{\upsilon}_{121}$ 1293.8 $\tilde{\upsilon}_{122}$ 1298.6 $\tilde{\upsilon}_{123}$ 1310.2 $\tilde{\upsilon}_{124}$ 1324.9 $\tilde{\upsilon}_{125}$ 1331.4 $\tilde{\upsilon}_{126}$ 1348.2 $\tilde{\upsilon}_{127}$ 1364.4 $\tilde{\upsilon}_{128}$ 1365.8 $\tilde{\upsilon}_{129}$ 1373.5 $\tilde{\upsilon}_{130}$ 1390.7 $\tilde{\upsilon}_{131}$ 1400.8 $\tilde{\upsilon}_{132}$ 1408.5 $\tilde{\upsilon}_{133}$ 1427.7 $\tilde{\upsilon}_{134}$ 1428.9 $\tilde{\upsilon}_{135}$ 1432 $\tilde{\upsilon}_{136}$ 1433 $\tilde{\upsilon}_{137}$ 1466.8 $\tilde{\upsilon}_{138}$ 1472.2 $\tilde{\upsilon}_{139}$ 1481.3 $\tilde{\upsilon}_{140}$ 1482.1 $\tilde{\upsilon}_{141}$ 1486.3 $\tilde{\upsilon}_{142}$ 1488.9 $\tilde{\upsilon}_{143}$ 1494.2 $\tilde{\upsilon}_{144}$ 1498.3 $\tilde{\upsilon}_{145}$ 1501.6 $\tilde{\upsilon}_{146}$ 1503.6 $\tilde{\upsilon}_{147}$ 1505.2 $\tilde{\upsilon}_{148}$ 1506.9 $\tilde{\upsilon}_{149}$ 1512.6 $\tilde{\upsilon}_{150}$ 1516.5 $\tilde{\upsilon}_{151}$ 1523.1 $\tilde{\upsilon}_{152}$ 1537.9 $\tilde{\upsilon}_{153}$ 1563.1 $\tilde{\upsilon}_{154}$ 1581.4 $\tilde{\upsilon}_{155}$ 2889.8 $\tilde{\upsilon}_{156}$ 2920.7 $\tilde{\upsilon}_{157}$ 2926.9 $\tilde{\upsilon}_{158}$ 2935.3 $\tilde{\upsilon}_{159}$ 2940.3 $\tilde{\upsilon}_{160}$ 2943.3 $\tilde{\upsilon}_{161}$ 2944.7 $\tilde{\upsilon}_{162}$ 2951 $\tilde{\upsilon}_{163}$ 2959.9 $\tilde{\upsilon}_{164}$ 2972.2 $\tilde{\upsilon}_{165}$ 2973.4 $\tilde{\upsilon}_{166}$ 2988.7 $\tilde{\upsilon}_{167}$ 2998.5 $\tilde{\upsilon}_{168}$ 2999.6 $\tilde{\upsilon}_{169}$ 3003.9 $\tilde{\upsilon}_{170}$ 3010.9 $\tilde{\upsilon}_{171}$ 3015.1 $\tilde{\upsilon}_{172}$ 3016.3 $\tilde{\upsilon}_{173}$ 3021.5 $\tilde{\upsilon}_{174}$ 3039.8 $\tilde{\upsilon}_{175}$ 3055.9 $\tilde{\upsilon}_{176}$ 3061.3 $\tilde{\upsilon}_{177}$ 3063.5 $\tilde{\upsilon}_{178}$ 3069.8 $\tilde{\upsilon}_{179}$ 3076.1 $\tilde{\upsilon}_{180}$ 3078.3 $\tilde{\upsilon}_{181}$ 3090.5 $\tilde{\upsilon}_{182}$ 3117.2 $\tilde{\upsilon}_{183}$ 3115.3.

Table S6.6 Comparison of calculated and reported value of $C_{11}=C_{12}$ stretching frequency and frequency of wagging motion in HOOP region in the following systems.

System	$-C_{11}=C_{12}$ stretching frequency (cm^{-1})	Frequency of wagging motions in HOOP region (cm^{-1})
		For H–C_{11},C_{12} H bonds
11 cis retinal	1526	969
all trans retinal	1528	898,887,859
Rhodopsin	1548	969
Bathorhodopsin	1535	920,875,850
11 cis retinal-gold(O_h) conjugate	1513	965
all-trans retinal-gold(O_h) conjugate	1506	903,864,837
11 cis retinal-gold(D_{2h}) conjugate	1507	965
all-trans retinal-gold(D_{2h}) conjugate	1467	905,846,836