Supplementary Material: Calculated linear and nonlinear optical absorption spectra of phosphine-ligated gold clusters

Paul N. Day,[a,b][*] Ruth Pachter,[a][*] Kiet A. Nguyen[a,b]

[a]Air Force Research Laboratory, Materials and Manufacturing Directorate,

Wright-Patterson Air Force Base, OH 45433, USA

[b]UES, Inc. Dayton OH 45432, USA

Table S1. Comparison of calculated excited-state energies for $Au_8(PR_3)_7^{2+}$, R = Ph, with comparison to the Voigt-function resolved features from the measured H.R. absorption spectrum. The primary orbital transition in our calculations is listed in the last two rows.

												MUE
measured[1]	2.06	2.26	2.42	2.68	2.76	2.92	3.05	3.09	3.36	3.41	3.49	
TD-PBE0	2.19	2.41	2.70	2.92	2.95	3.02	3.15	3.21	3.25	3.31	3.34	**0.15**
G0W0-PBE0	1.90	2.12	2.45	2.65	2.70	2.76	2.89	2.95	2.96	3.01	3.11	**0.19**
evGW-PBE0	2.08	2.29	2.63	2.82	2.87	2.94	3.07	3.12	3.13	3.18	3.28	**0.11**
TD-CAM	2.39	2.67	3.02	3.27	3.32	3.47	3.57	3.68	3.69	3.78	3.91	**0.48**
G0W0-CAM	2.16	2.43	2.79	3.02	3.05	3.15	3.28	3.37	3.39	3.51	3.59	**0.20**
evGW-CAM	2.13	2.41	2.77	2.99	3.02	3.13	3.26	3.35	3.37	3.49	3.57	**0.18**
TD-B3LYP	2.10	2.32	2.61	2.82	2.85	2.90	3.01	3.07	3.14	3.14	3.17	**0.13**
evGW-B3LYP	2.06	2.28	2.62	2.81	2.86	2.93	3.04	3.10	3.12	3.15	3.24	**0.11**
TD-PBE	1.86	1.98	2.24	2.36	2.40	2.43	2.47	2.49	2.51	2.56	2.57	**0.51**
evGW-PBE	2.01	2.14	2.50	2.64	2.71	2.75	2.77	2.81	2.85	2.89	2.90	**0.24**
Orb. Trans.	H	H-1	H	H-1	H	H	H	H-1	H-1	H-2	H-1	
	L	L	L+1	L+1	L+2	L+3	L+4	L+2	L+2	L	L+4	

Table S2. Measured and calculated absorption features for $Au_9(PR_3)_8{}^{3+}$ with R = Ph. Measured data in the solvents methanol (MeOH), acetonitrile (ACN), and dichloromethane (DCM), and in a thin-film of poly(methyl methacrylate) (PMMA). The final section has results for the average of the two structures. The mean-unsigned-error (MUE) is for the first five features, relative to the high-resolution measurement.

measurement	solvent											MUE
High-res. UV-Vis[2]		2.04	2.45	2.73	2.87	3.07	3.38	3.60	3.80	3.91	4.06	
UV-Vis[2]	MeOH	1.97	2.42		2.80	3.00	3.26	3.53	3.75			
UV-Vis[3]	ACN				2.80		3.27	3.59		3.95		
UV-Vis[4]	PMMA	2.38	2.62		2.79	2.99		3.58				
UV-Vis[5]	DCM				2.81		3.32	3.60		3.92		
UV-Vis[5]	MeOH				2.80		3.27	3.51		3.92		
theory: D_2												**MUE**
TD-LB94[6]		1.66	2.21	2.47	3.10	3.37						
TD-GRAC[1]		1.57	2.27	2.43								
TD-PBE0		1.93	2.43	2.90	3.11	3.42	3.61	3.71	3.95			**0.18**
evGW-BSE:PBE0		1.82	2.31	2.79	3.00	3.33		3.54	3.69			**0.16**
evGW-BSE:CAM		1.88	2.47	2.95	3.25	3.54	3.75	3.95	4.16	4.29		**0.25**
theory: C_4												
SO-TDDFT[5]	DCM				2.93	3.15	3.37			4.21		
SO-TDDFT[5]	MeOH				2.93	3.15	3.37			4.21		
TD-PBE0			2.35	2.75	2.93		3.44	3.63	3.80	3.93		
evGW-BSE:PBE0			2.27	2.65	2.83		3.34			3.81		
evGW-BSE:CAM			2.30	2.68	2.89		3.41	3.64	3.77	3.98		
Ave.(D_2-C_4)												**MUE**
TD-PBE0		1.93	2.43	2.75	2.93	3.11	3.43	3.61	3.71	3.94		**0.05**
evGW-BSE:PBE0		1.82	2.30	2.65	2.83	3.00	3.34	3.54	3.69	3.78		**0.11**
evGW-BSE:CAM		1.88	2.47	2.68	2.90	3.25	3.42	3.64	3.74	3.95		**0.09**

Table S3. Comparison of calculated excited-state energies for $Au_9(PR_3)_8^{3+}$, R = Ph, with comparison to the Voigt-function resolved features[1] from the measured H.R. absorption spectrum.

												MUE
measured[1]	2.06	2.44	2.50	2.68	2.75	2.86	2.90	3.08	3.17	3.34	3.39	
TD-PBE0,D_2	1.93	2.20	2.43	2.73	2.90	3.08	3.11	3.17	3.21	3.30	3.34	**0.12**
evGW:PBE0,D_2	1.82	2.13	2.30	2.63	2.79	2.96	3.00	3.06	3.09	3.19	3.21	**0.13**
TD-PBE0,C_4	2.35	2.35	2.75	2.75	2.93	2.93	3.34	3.34	3.39	3.43	3.43	**0.18**
evGW:PBE0,C_4	2.27	2.27	2.65	2.65	2.83	2.83	3.25	3.25	3.28	3.34	3.34	**0.12**

Table S4. Orbital and transition energies (eV) for the first singlet excited state, S1. The vertical absorption (V.A.) energy is the energy difference between the S0 and S1 states at the S0-optimized geometry, the vertical emission (V.E.) energy is the difference at the S1-optimized geometry, and ΔE is the difference between the minima. H-L denotes the HOMO-LUMO gap. For the Au$_9$ systems, results are for the D$_2$ isomer. Hammett parameters for the ligand substituents and calculated Mulliken charges (M.C.) on the central gold atom are also given.

Au$_9$(PR$_3$)$_8$$^{3+}$	R = Ph	R = PhCH$_3$	R = PhOCH$_3$	R = PhNH$_2$	R = PhNO$_2$
Hammett	0.000	-0.170	-0.268	-0.660	0.778
M.C. Au(1)	-1.681	-1.687	-1.789	-1.759	-1.955
HOMO	-10.410	-9.978	-9.690	-9.114	-12.316
LUMO	-7.640	-7.232	-6.996	-6.411	-9.537
H-L	2.770	2.746	2.694	2.703	2.779
TDDFT:ver.Abs.	1.931	1.907	1.869	1.917	1.951
TDDFT:DE	1.595				
TDDFT:ver.emit	1.222				
HOMO(evGW)	-10.580	-10.130	-9.850	-9.357	
LUMO(evGW)	-6.470	-6.100	-5.880	-5.268	
H-L (evGW	4.110	4.030	3.970	4.089	
evGW-BSE:ver.Abs.	1.820	1.804	1.790	1.935	
measured	2.037	1.927	1.829		

Au$_8$(PR$_3$)$_7$$^{2+}$	R = Ph	R = PhCH$_3$	R = PhOCH$_3$
Hammett	0.000	-0.170	-0.268
M.C. Au(1)	-1.399	-1.446	-1.723
HOMO	-8.471	-8.099	-7.955
LUMO	-5.464	-5.092	-5.007
H-L	3.007	3.007	2.948
TDDFT:ver.Abs.	2.188	2.193	2.132
TDDFT:DE	1.697		
TDDFT:ver.emit	0.820		
HOMO(evGW)	-8.610	-8.270	-8.130
LUMO(evGW)	-3.950	-3.900	-3.850
H-L (evGW	4.660	4.370	4.280
evGW-BSE:ver.Abs.	2.076	2.092	2.013
measured	2.068	2.010	1.961

Table S5. For the D_2 isomer of $Au_9(PR_3)_8^{3+}$, TD-PBE0 transition energies in eV (ΔE), oscillator strengths (O.S.), and the initial and final orbitals for the primary contribution to the excitation. The superatom character of the orbital is indicated where identified.

	R=Ph ΔE	R=Ph O.S.	R=Ph init.orb.	R=Ph fin.orb.	R=PhOMe ΔE	R=PhOMe O.S.	R=PhOMe init.orb.	R=PhOMe fin.orb.
1	1.9314	0.0375	HOMO (P_y)	LUMO (D_{x2-y2})	1.8686	0.0345	HOMO (P_y)	LUMO (D_{x2-y2})
2	2.2040	0.0000	HOMO (P_y)	L+1 (P_z)	2.1527	0.0000	HOMO (P_y)	L+1 (P_z)
3	2.4261	0.0040	H-1 (P_x)	LUMO (D_{x2-y2})	2.3589	0.0023	H-1 (P_x)	LUMO (D_{x2-y2})
4	2.7268	0.0006	H-1 (P_x)	L+1 (P_z)	2.6658	0.0009	H-1 (P_x)	L+1 (P_z)
5	2.9038	0.0160	HOMO (P_y)	L+2 (D_{xy})	2.7600	0.0047	H-2	LUMO (D_{x2-y2})
6	3.0753	0.0000	HOMO (P_y)	L+3 (F)	2.9470	0.2549	HOMO (P_y)	L+2 (D_{xy})
7	3.1110	0.2990	H-2	LUMO (D_{x2-y2})	2.9737	0.0018	H-4	LUMO (D_{x2-y2})
8	3.1690	0.0025	HOMO (P_y)	L+4 (D_{yz})	3.0138	0.0000	H-3	LUMO (D_{x2-y2})
9	3.2070	0.0088	H-3	LUMO (D_{x2-y2})	3.0149	0.0000	HOMO (P_y)	L+3 (F)
10	3.3048	0.0000	H-2	L+1 (P_z)	3.0409	0.0001	H-5	LUMO (D_{x2-y2})
11	3.3413	0.0000	H-5	LUMO (D_{x2-y2})	3.0884	0.0028	HOMO (P_y)	L+4 (D_{yz})
12	3.3498	0.0000	H-4	LUMO (D_{x2-y2})	3.1082	0.0016	H-2	L+1 (P_z)
13	3.4219	0.0479	H-1 (P_x)	L+2 (D_{xy})	3.1809	0.0000	H-6	LUMO (D_{x2-y2})
14	3.4999	0.0000	H-3	L+1 (P_z)	3.2230	0.0092	H-7	LUMO (D_{x2-y2})
15	3.5364	0.0001	HOMO (P_y)	L+5	3.2816	0.0000	H-4	L+1 (P_z)
16	3.5485	0.0000	H-6	LUMO (D_{x2-y2})	3.3297	0.0646	H-1 (P_x)	L+2 (D_{xy})
17	3.5575	0.0003	H-1 (P_x)	L+3 (F)	3.3583	0.1610	H-3	L+1 (P_z)
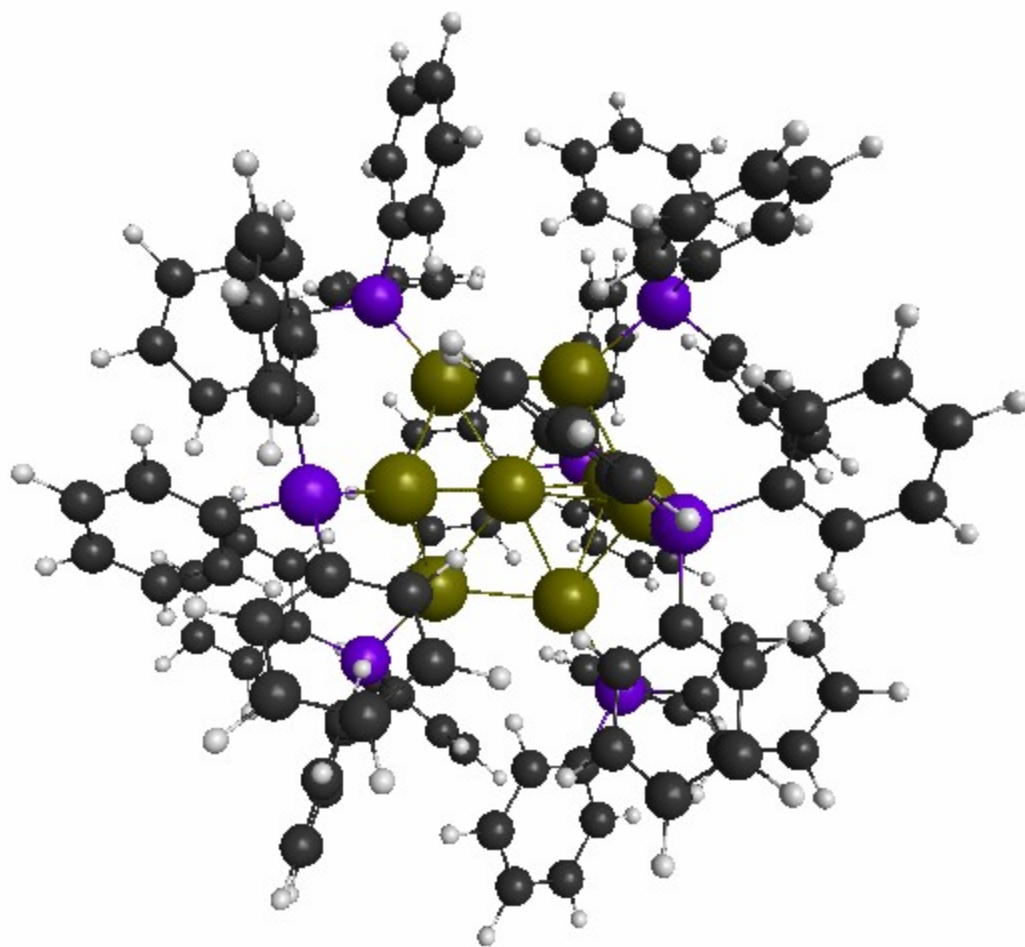
a) $Au_8(PR_3)_7^{2+}$, R=Ph
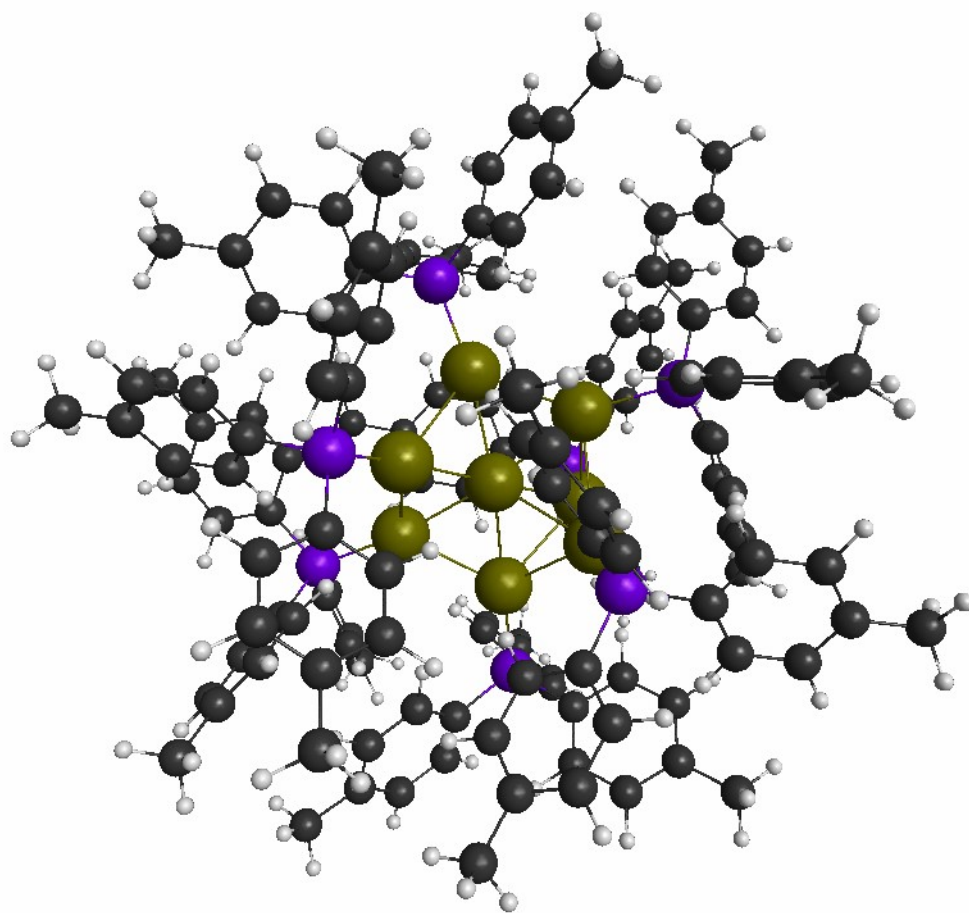
b) $Au_8(PR_3)_7^{2+}$, R=PhMe
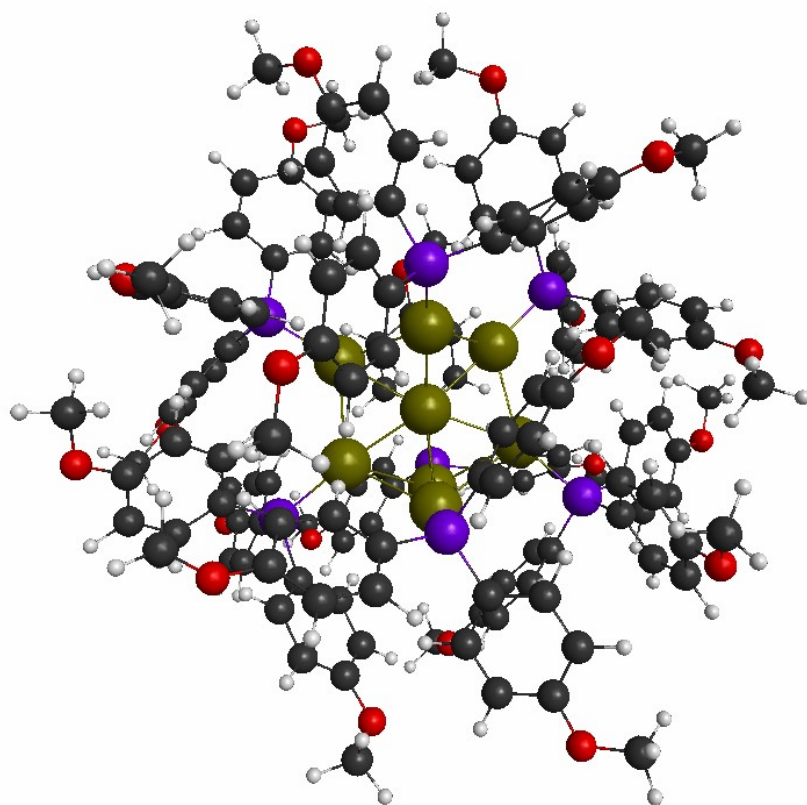
c) $Au_8(PR_3)_7^{2+}$, R=PhOMe
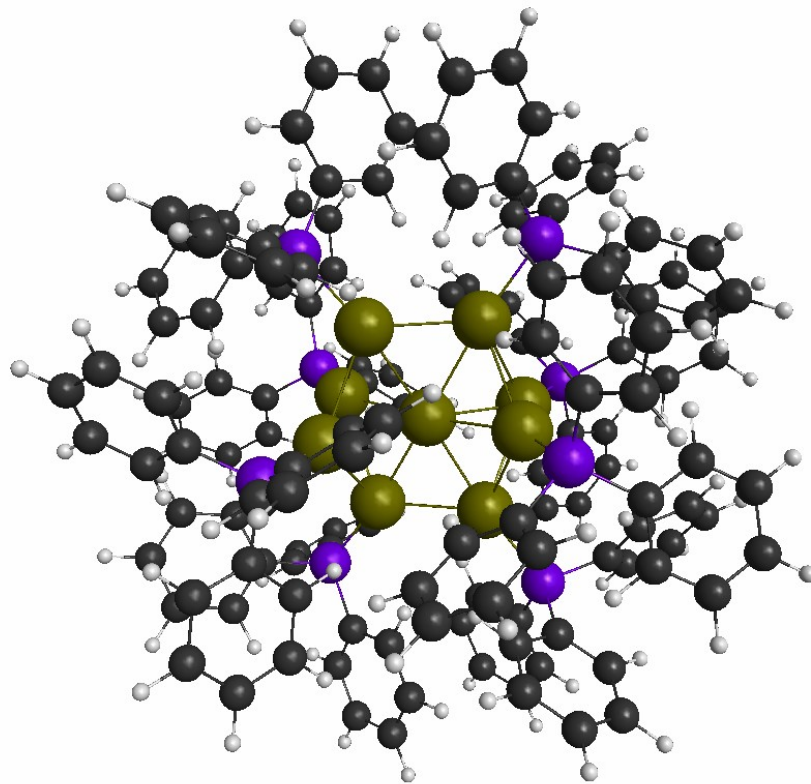
d) D_2 $Au_9(PR_3)_8^{3+}$, R=Ph
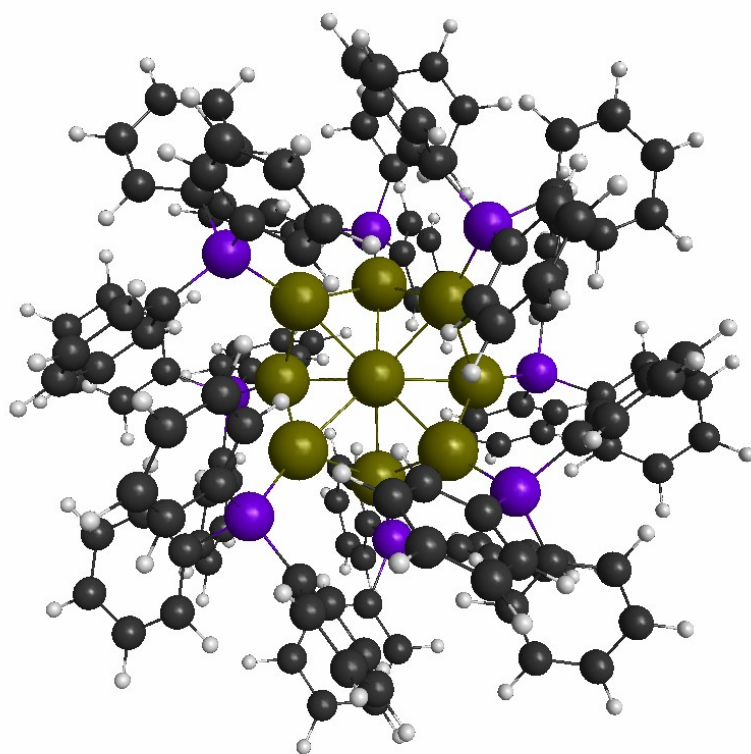
e) C_4 $Au_9(PR_3)_8^{3+}$, R=Ph
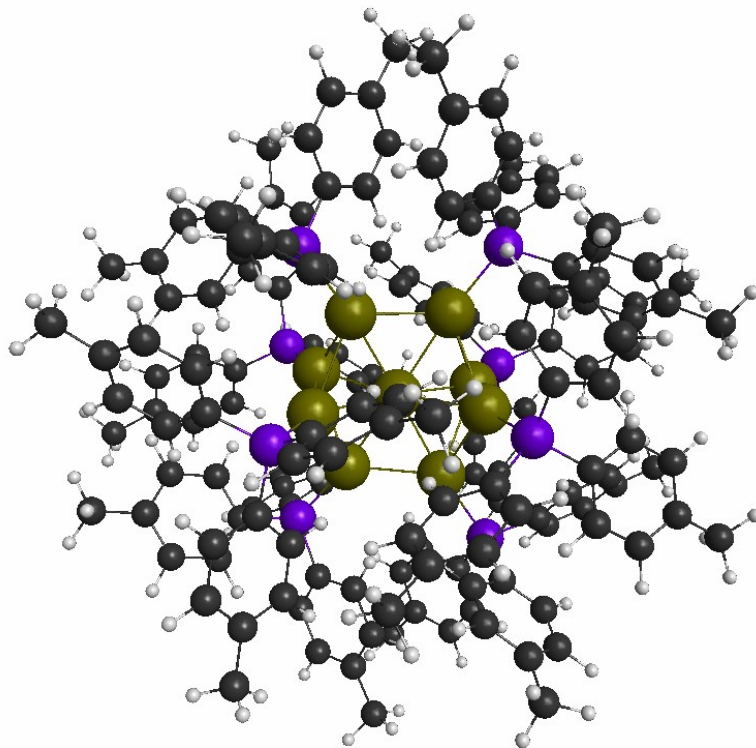
f) D_2 $Au_9(PR_3)_8^{3+}$, R=PhMe
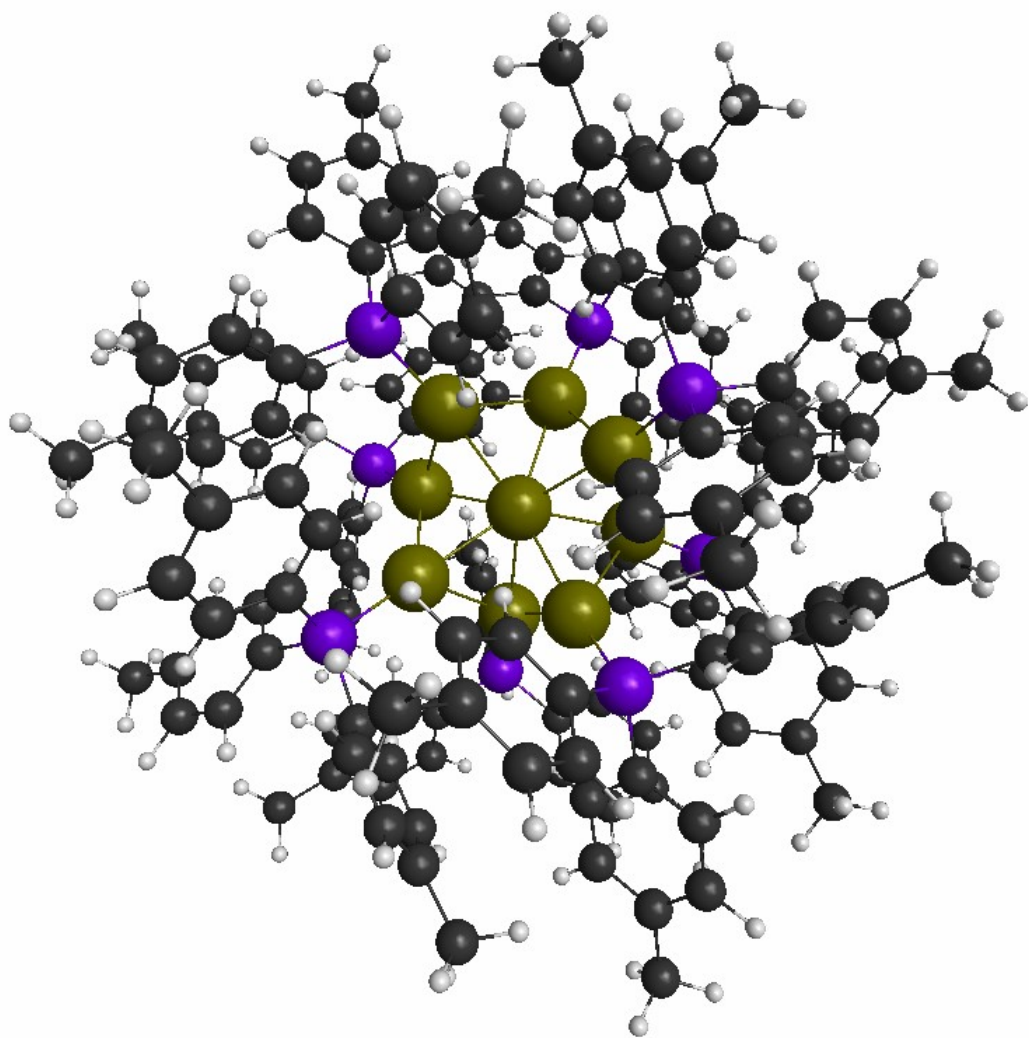
g) C_4 $Au_9(PR_3)_8^{3+}$, R=PhMe
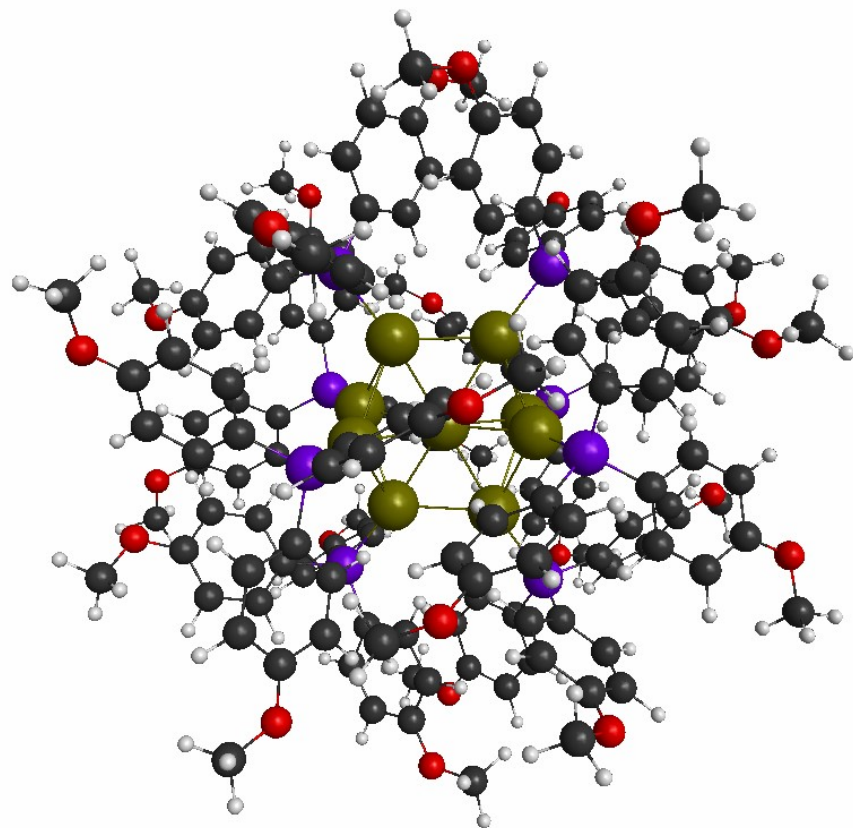
h) D_2 $Au_9(PR_3)_8^{3+}$, R=PhOMe
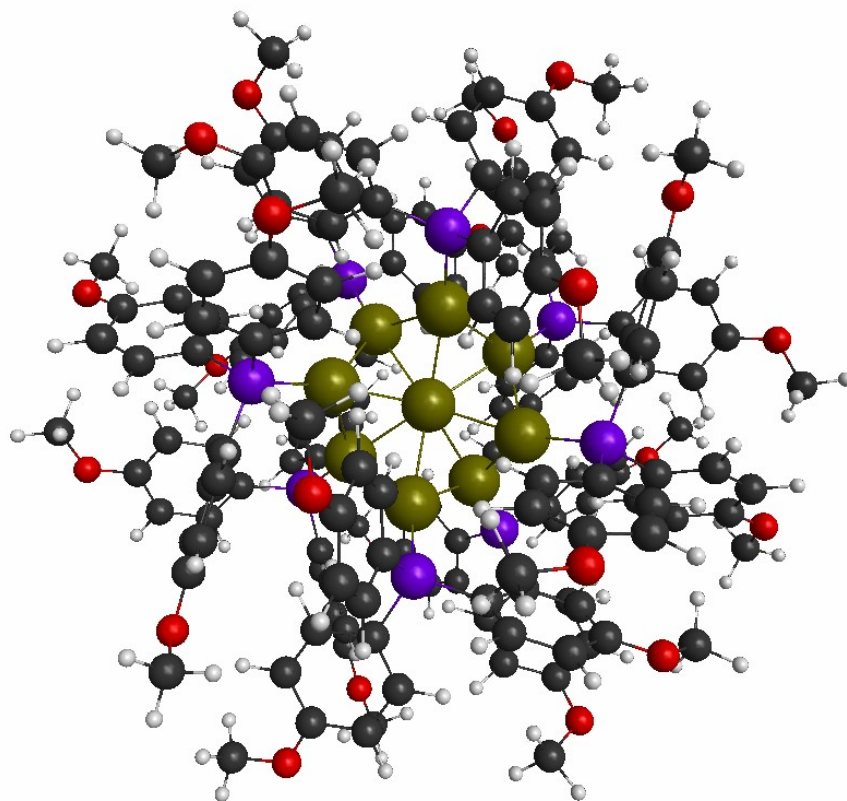
i) C_4 $Au_9(PR_3)_8{}^{3+}$, R=PhOMe

Figure S1. Structure of clusters studied.
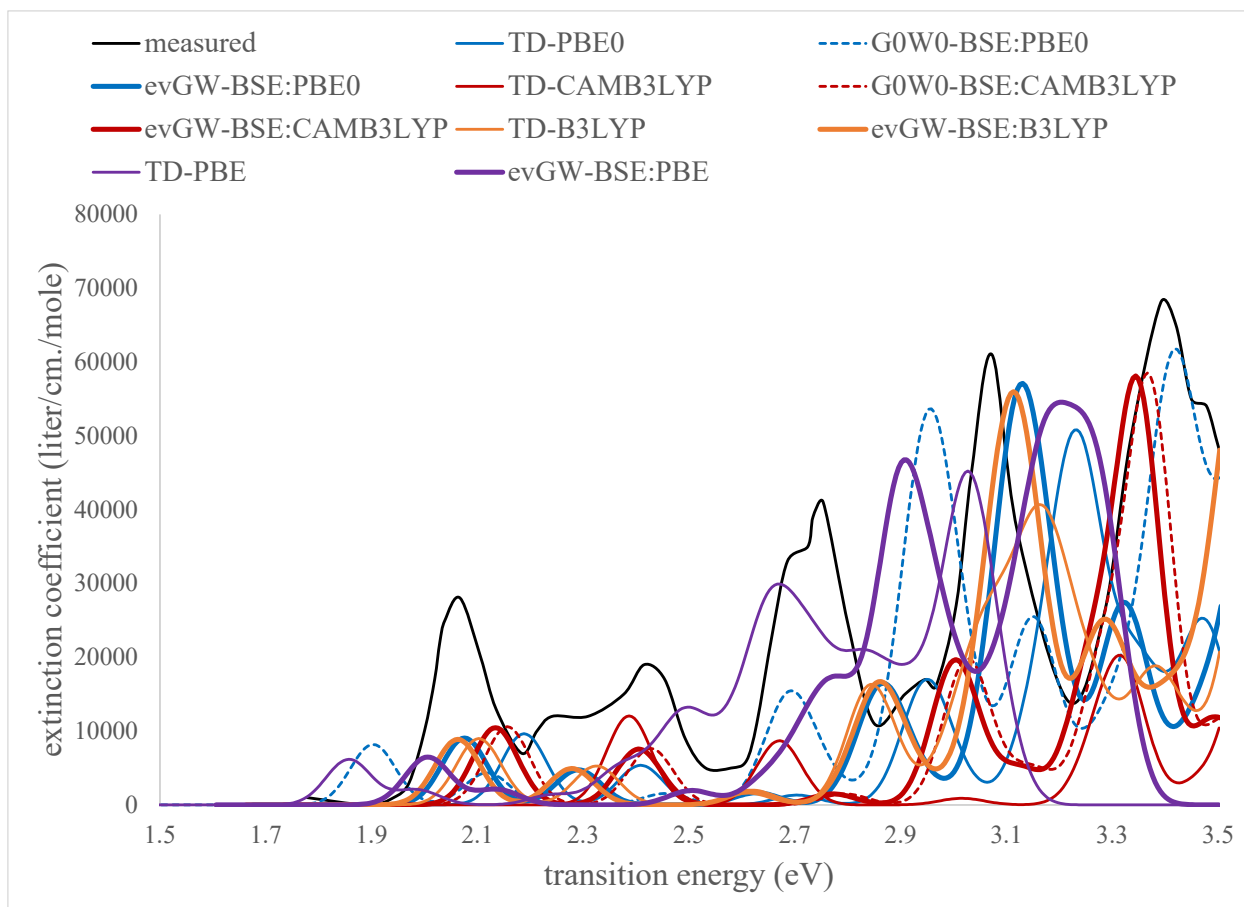
Figure S2. OPA calculated for $Au_8(PR_3)_7^{2+}$ when R = Ph at a geometry optimized with PBE0-D3, with comparison to experiment.[2] The extinction coefficients were calculated by fitting the calculated oscillator strengths to Gaussian functions with FWHM = 0.1 eV. The absolute intensity of the experimental spectra is arbitrary.
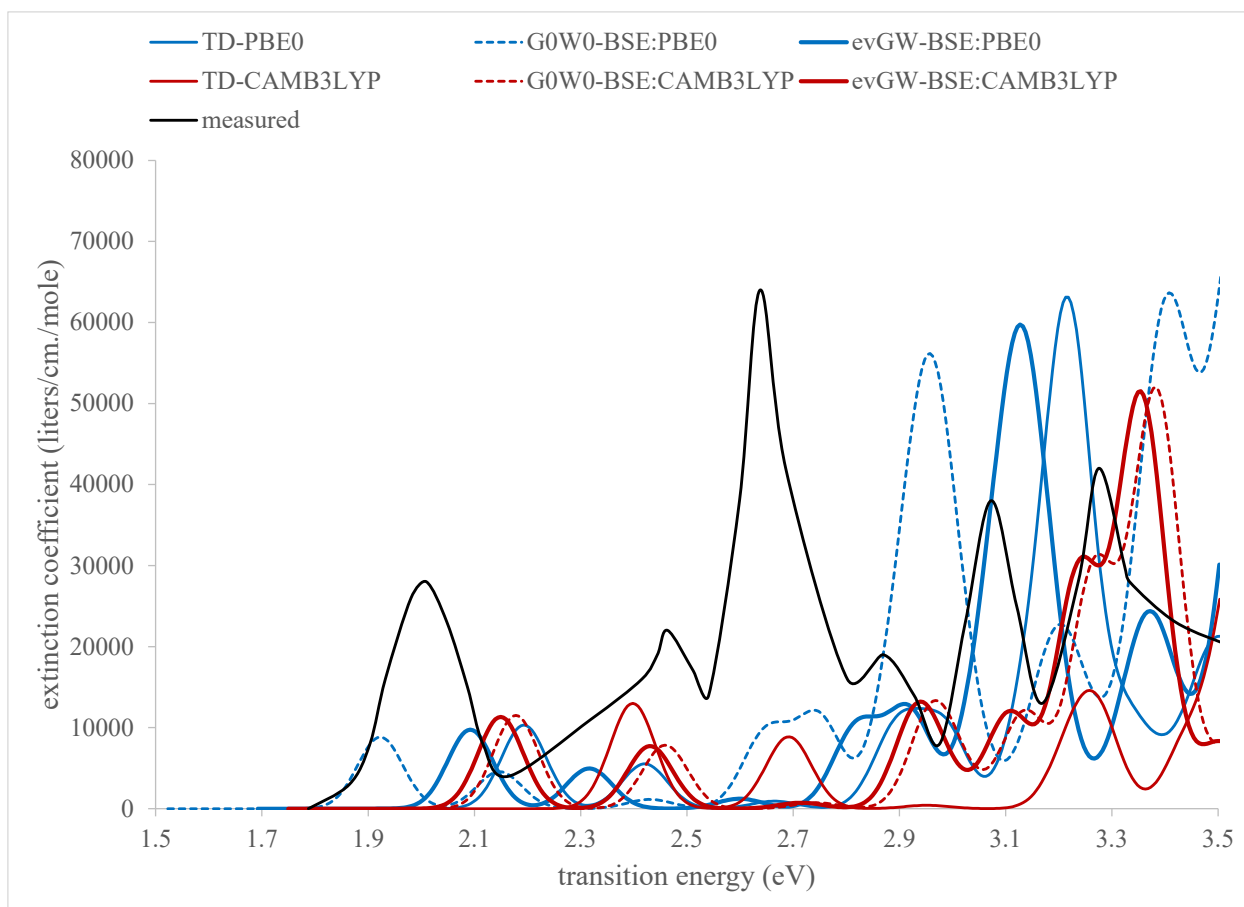
Figure S3. OPA calculated for $Au_8(PR_3)_7^{2+}$ when R = PhMe at a geometry optimized with PBE0-D3, with comparison to experiment.[2] The extinction coefficients were calculated by fitting the calculated oscillator strengths to Gaussian functions with FWHM = 0.1 eV. The absolute intensity of the experimental spectra is arbitrary.
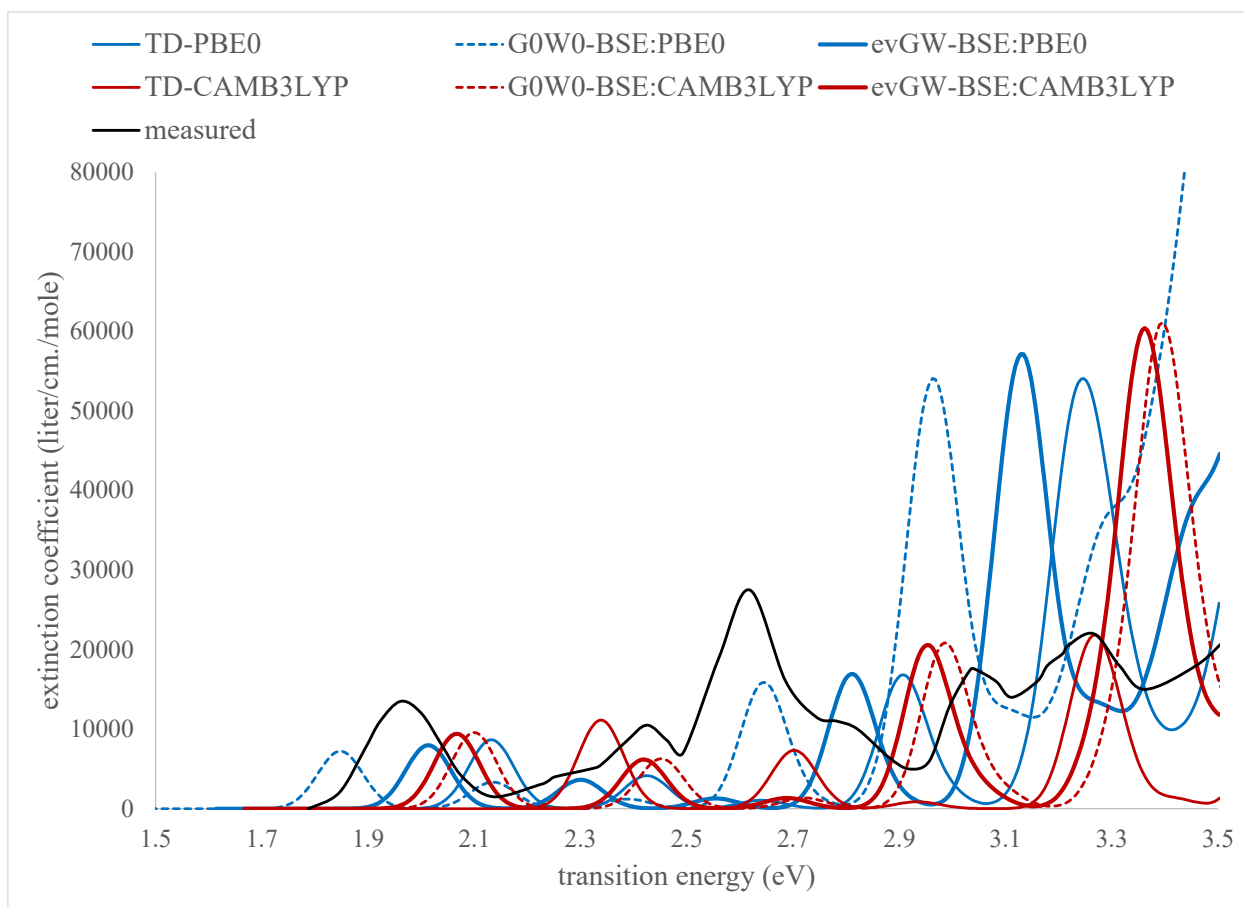
Figure S4. OPA calculated for $Au_8(PR_3)_7^{2+}$ when R = PhOMe at a geometry optimized with PBE0-D3, with comparison to experiment.[2] The extinction coefficients were calculated by fitting the calculated oscillator strengths to Gaussian functions with FWHM = 0.1 eV. The absolute intensity of the experimental spectra is arbitrary.
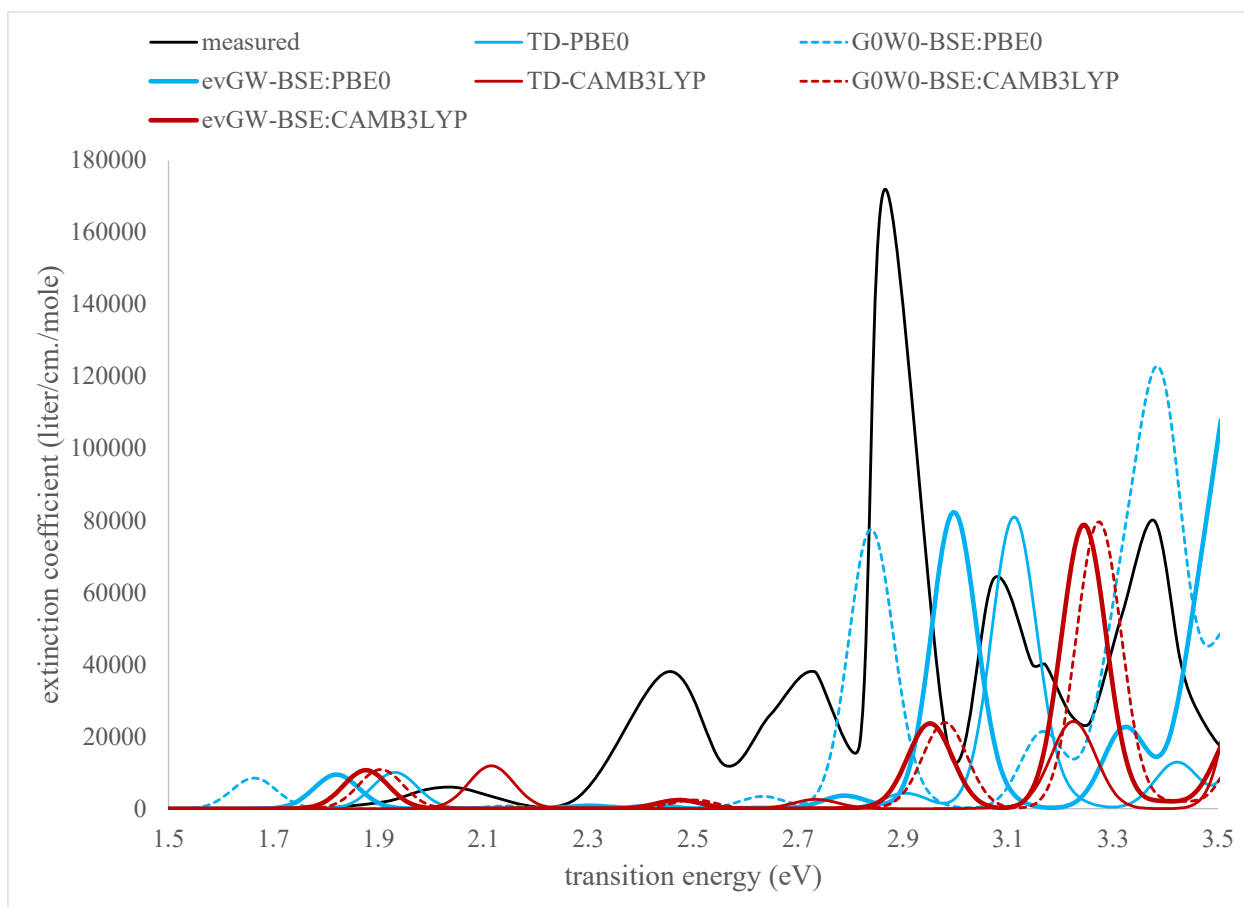
Figure S5. OPA calculated for D_2 $Au_9(PR_3)_8{}^{3+}$ when R = Ph at a geometry optimized with PBE0-D3, with comparison to experiment.[2] The extinction coefficients were calculated by fitting the calculated oscillator strengths to Gaussian functions with FWHM = 0.1 eV. The absolute intensity of the experimental spectra is arbitrary.
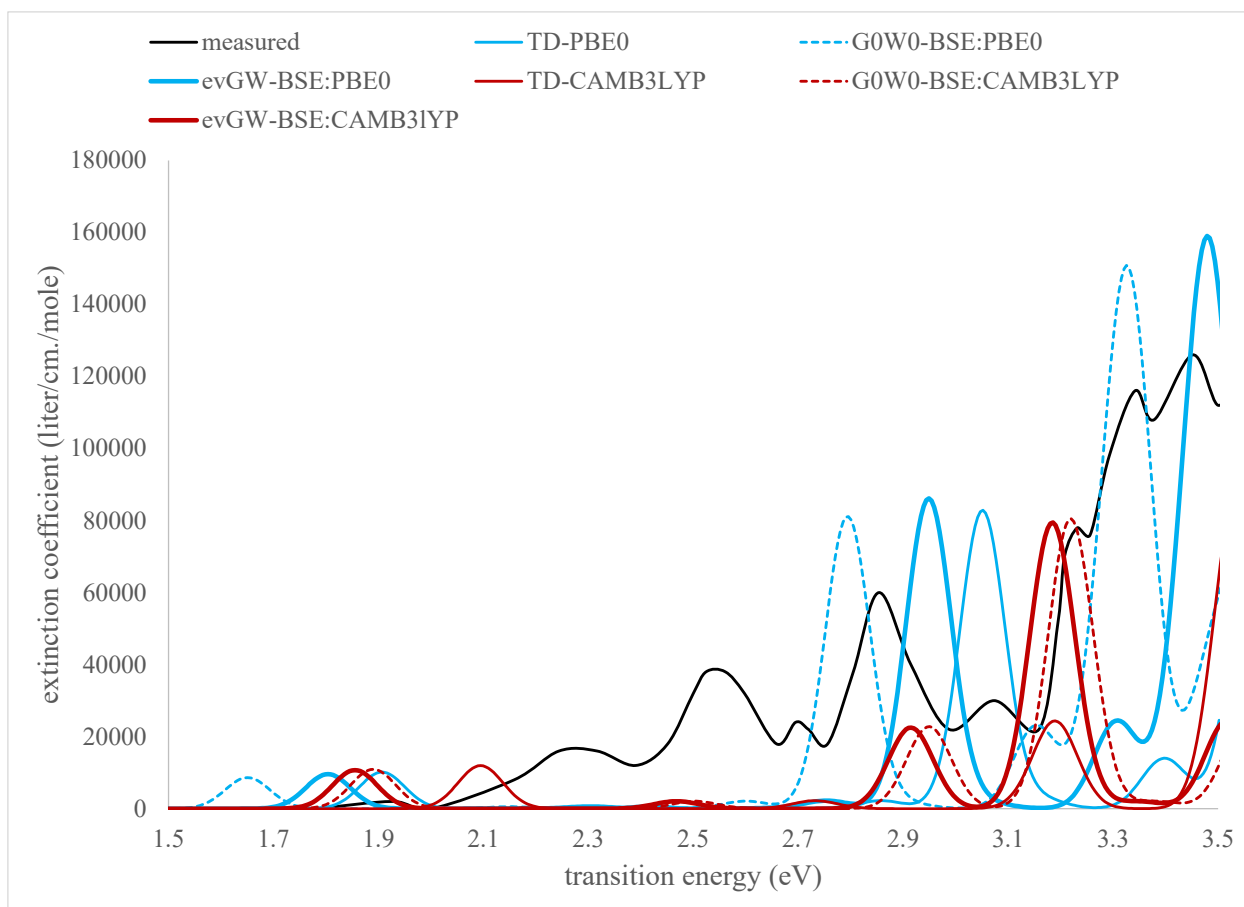
Figure S6. OPA calculated for D_2 $Au_9(PR_3)_8^{3+}$ when R = PhMe at a geometry optimized with PBE0-D3, with comparison to experiment.[2] The extinction coefficients were calculated by fitting the calculated oscillator strengths to Gaussian functions with FWHM = 0.1 eV. The absolute intensity of the experimental spectra is arbitrary.
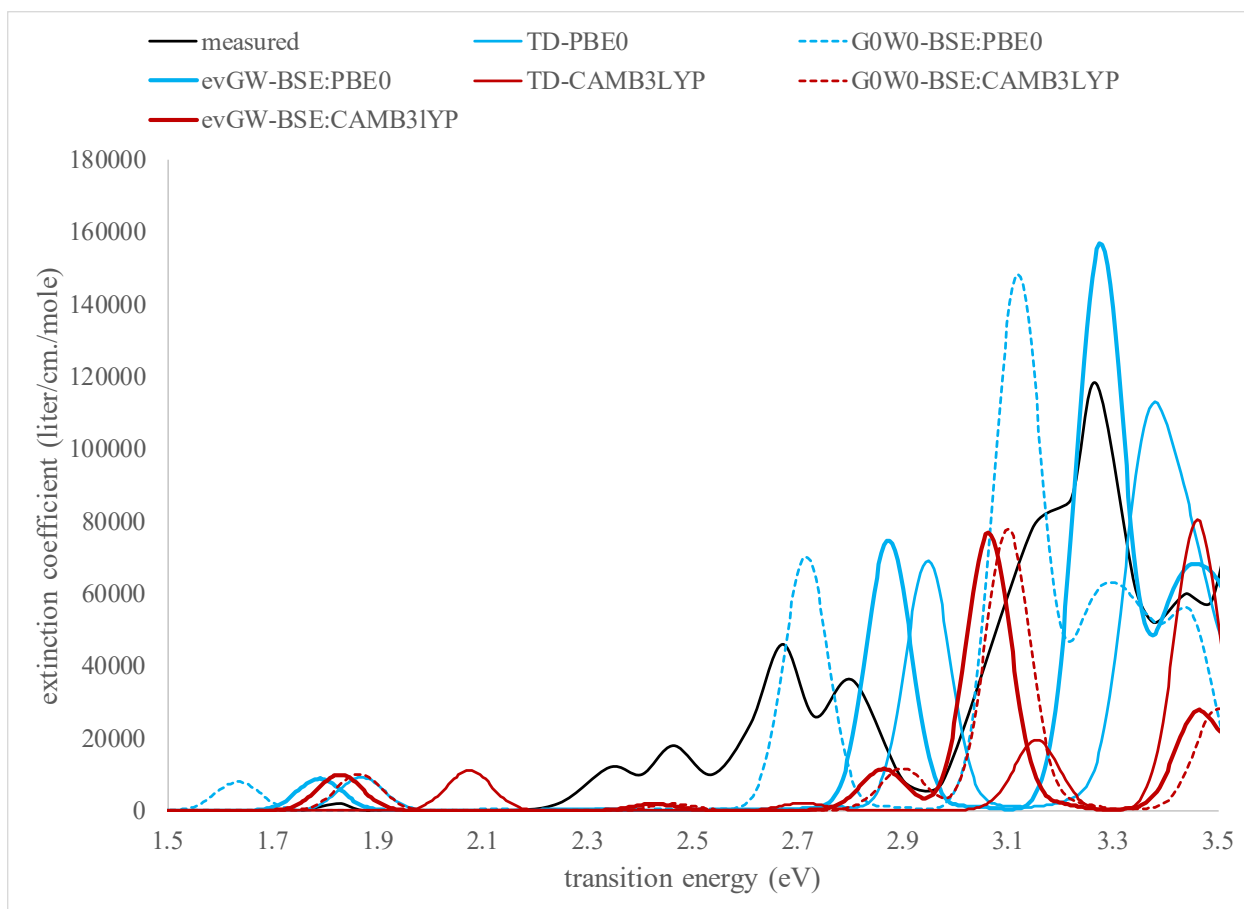
Figure S7. OPA calculated for D_2 $Au_9(PR_3)_8^{3+}$ when R = PhOMe at a geometry optimized with PBE0-D3, with comparison to experiment.[2] The extinction coefficients were calculated by fitting the calculated oscillator strengths to Gaussian functions with FWHM = 0.1 eV. The absolute intensity of the experimental spectra is arbitrary.
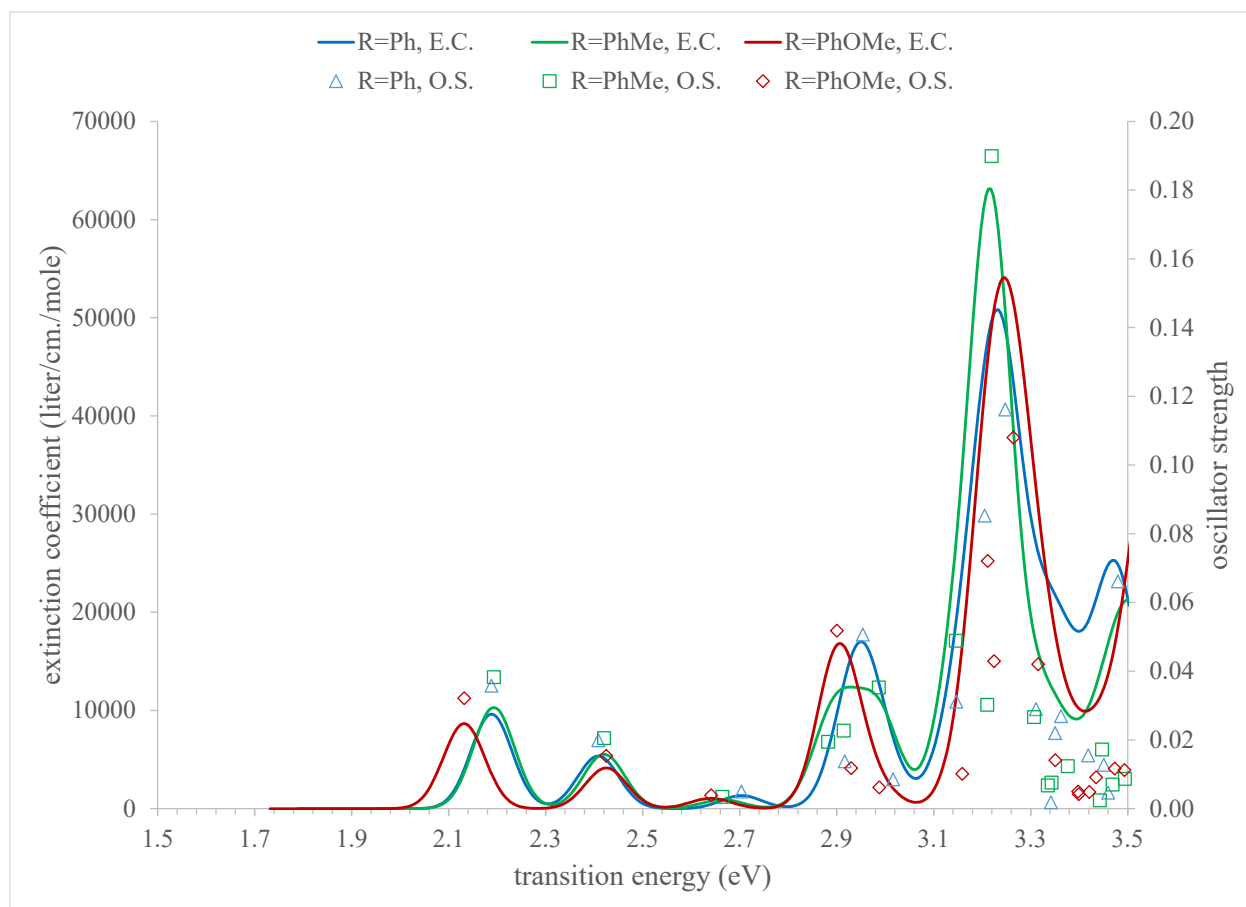
Figure S8. The effects of the ligands on the OPA of $Au_8(PR_3)_7{}^{2+}$ calculated using TD-PBE0. The oscillator strengths (O.S.) are plotted against the right vertical axis, while extinction coefficients (E.C.) were obtained by fitting to Gaussian linewidth functions with full-width at half-maximum of 0.1 eV.
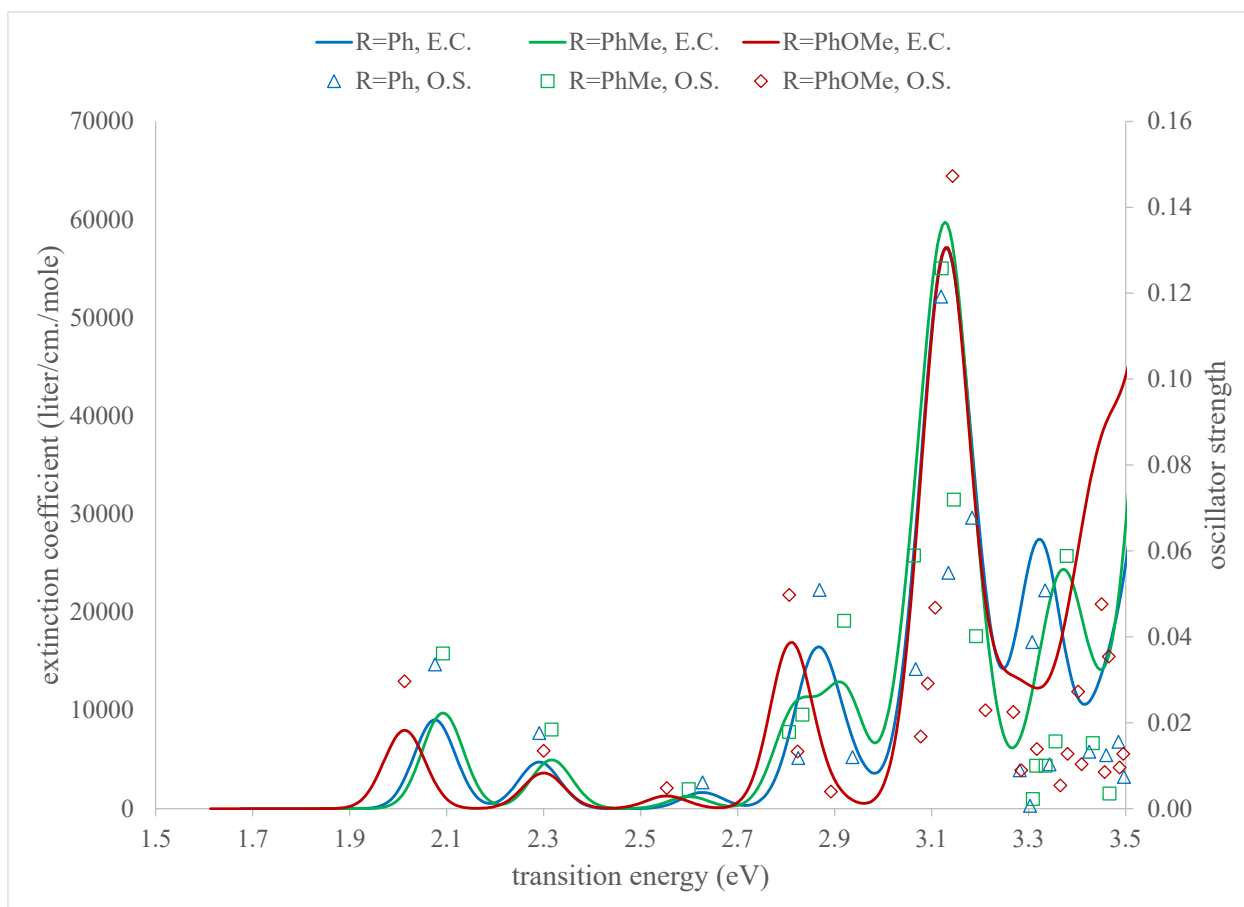
Figure S9. The effects of the ligands on the OPA of $Au_8(PR_3)_7^{2+}$ calculated using evGW-BSE:PBE0. The oscillator strengths (O.S.) are plotted against the right vertical axis, while extinction coefficients (E.C.) were obtained by fitting to Gaussian linewidth functions with full-width at half-maximum of 0.1 eV.
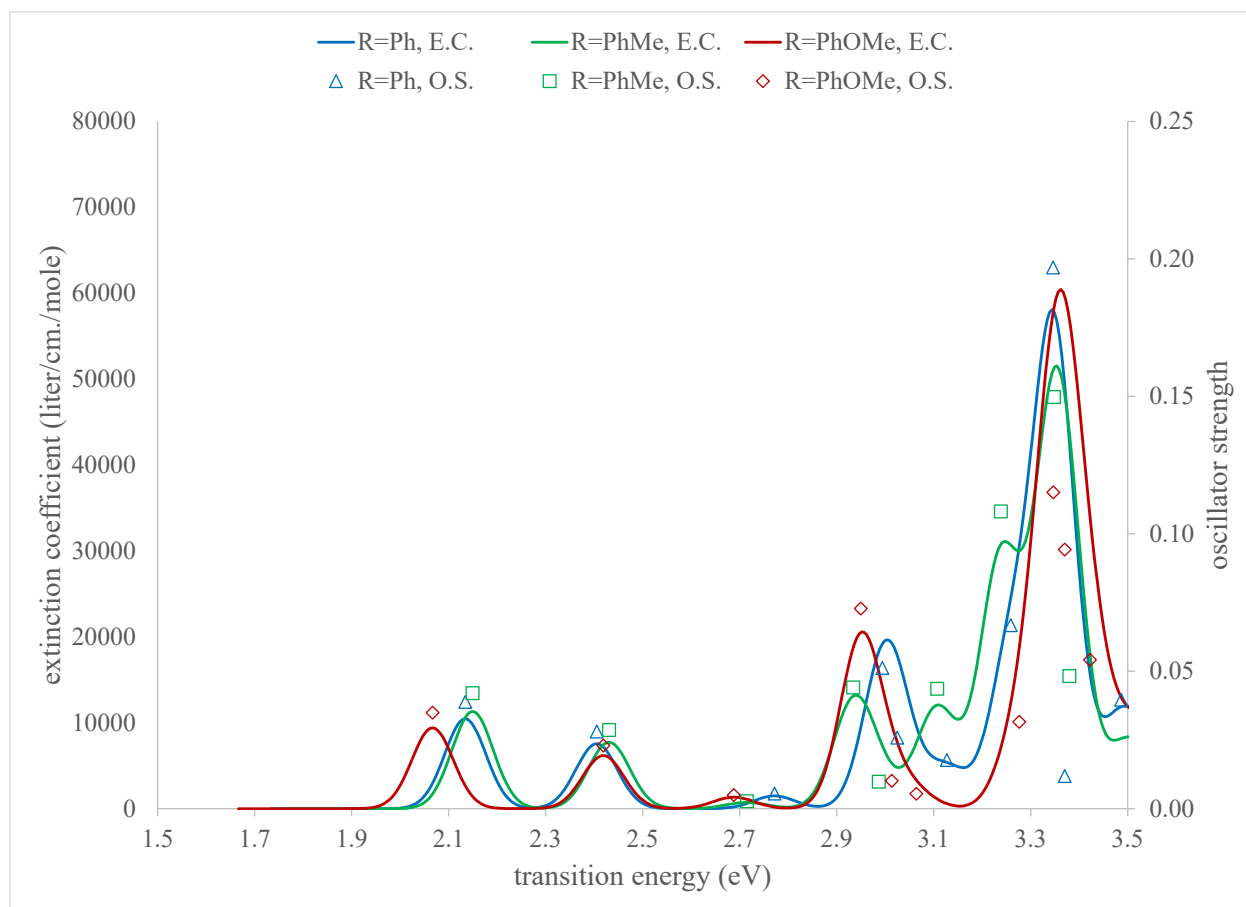
Figure S10. The effects of the ligands on the OPA of $Au_8(PR_3)_7{}^{2+}$ calculated using evGW-BSE:CAMB3LYP. The oscillator strengths (O.S.) are plotted against the right vertical axis, while extinction coefficients (E.C.) were obtained by fitting to Gaussian linewidth functions with full-width at half-maximum of 0.1 eV.
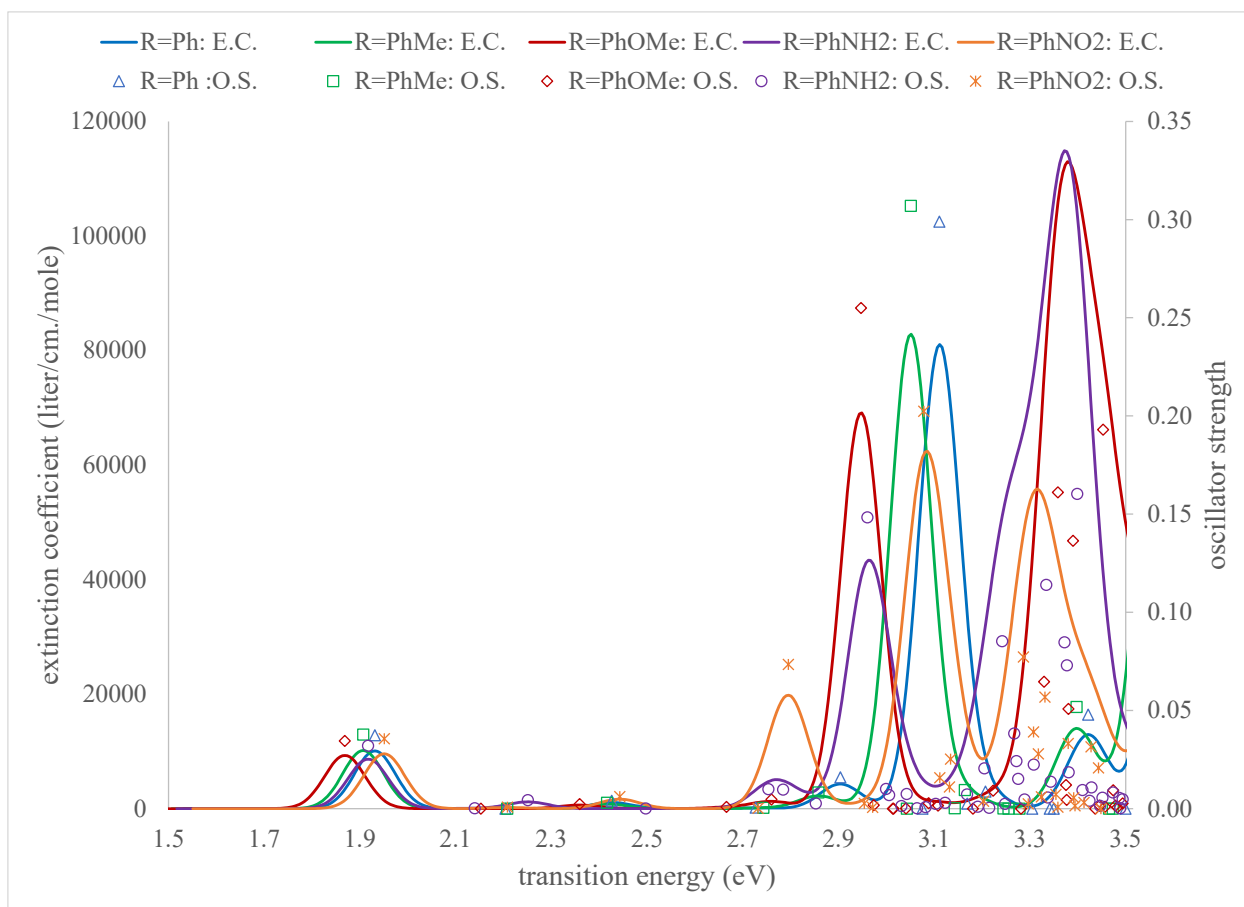
Figure S11. The effects of the ligands on the OPA of D_2 $Au_9(PR_3)_8{}^{3+}$ calculated using TD-PBE0. The oscillator strengths (O.S.) are plotted against the right vertical axis, while extinction coefficients (E.C.) were obtained by fitting to Gaussian linewidth functions with full-width at half-maximum of 0.1 eV.
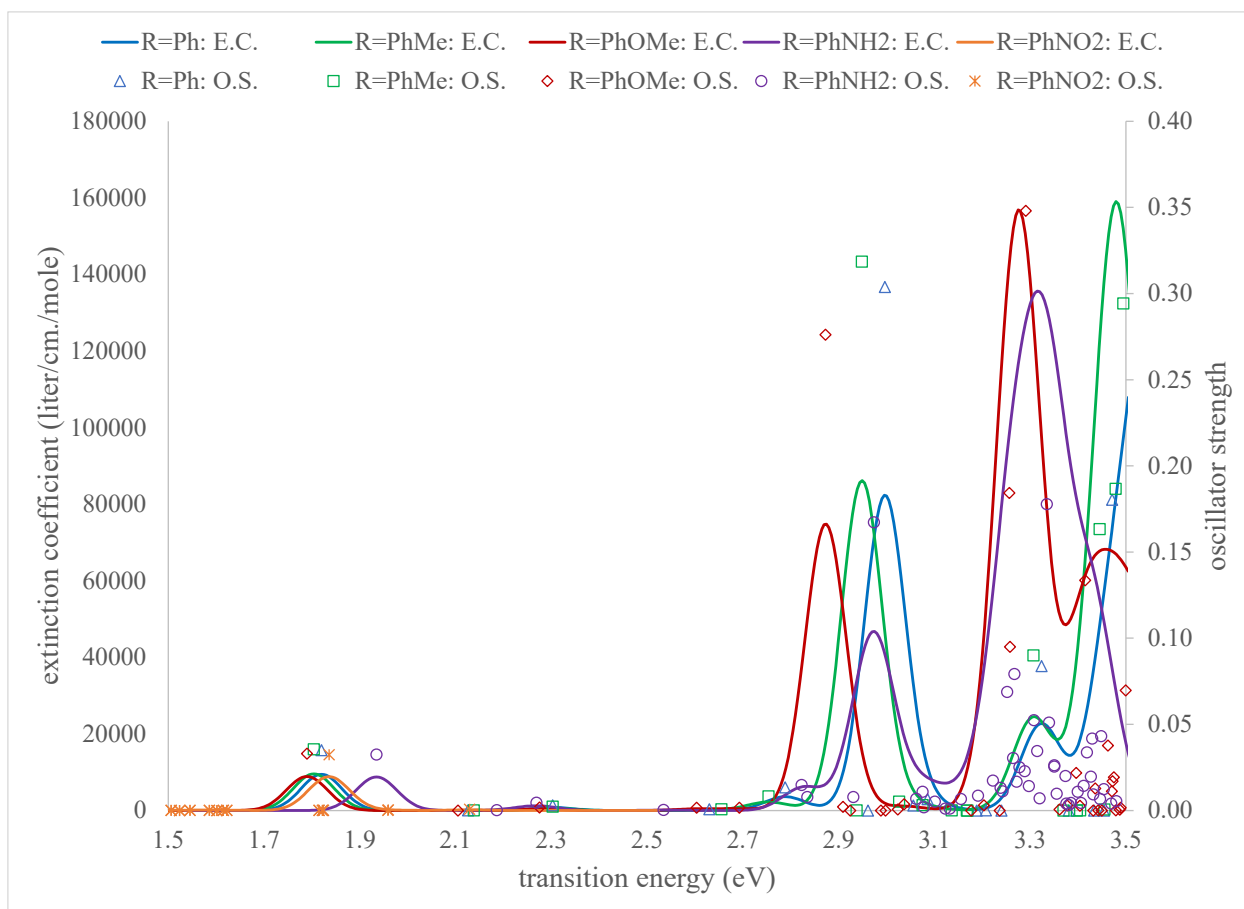
Figure S12. The effects of the ligands on the OPA of D_2 $Au_9(PR_3)_8^{3+}$ calculated using evGW-BSE:PBE0. The oscillator strengths (O.S.) are plotted against the right vertical axis, while extinction coefficients (E.C.) were obtained by fitting to Gaussian linewidth functions with full-width at half-maximum (FWHM) of 0.1 eV.
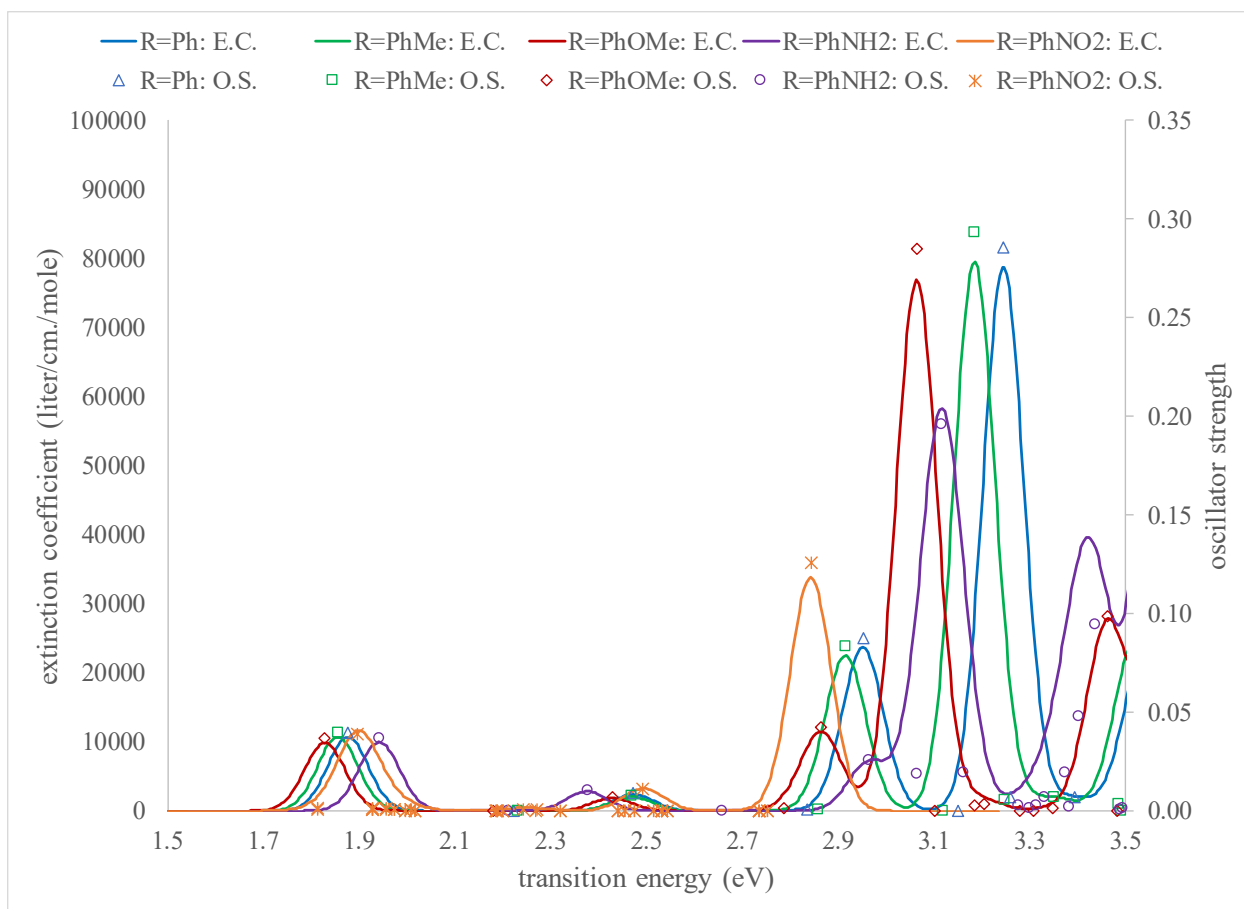
Figure S13. The effects of the ligands on the OPA of D_2 $Au_9(PR_3)_8{}^{3+}$ calculated using evGW-BSE:CAMB3LYP. The oscillator strengths (O.S.) are plotted against the right vertical axis, while extinction coefficients (E.C.) were obtained by fitting to Gaussian linewidth functions with full-width at half-maximum (FWHM) of 0.1 eV.
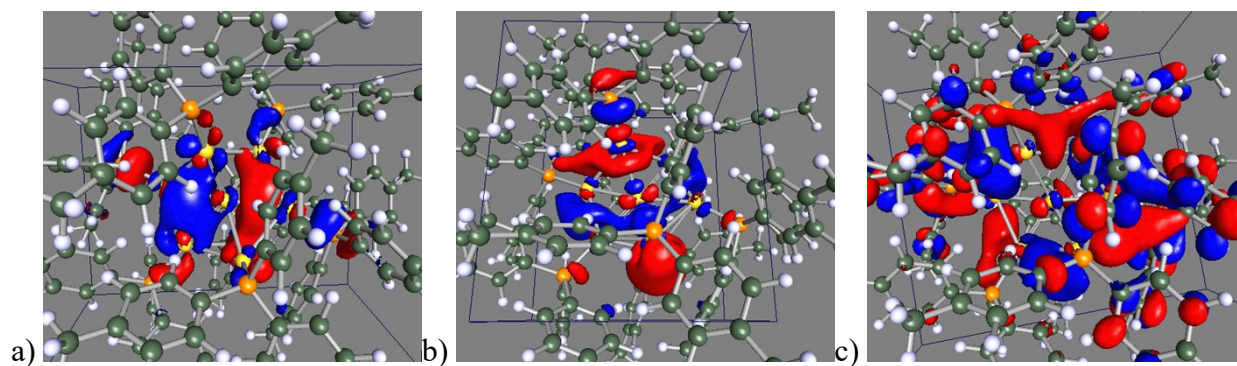
Figure S14. Key orbitals in the first TPA peak of $Au_8(PR_3)_7^{2+}$ with R = PhMe. a) HOMO with superatom P character. b) LUMO with superatom D character. c) LUMO+3 with superatom F character.
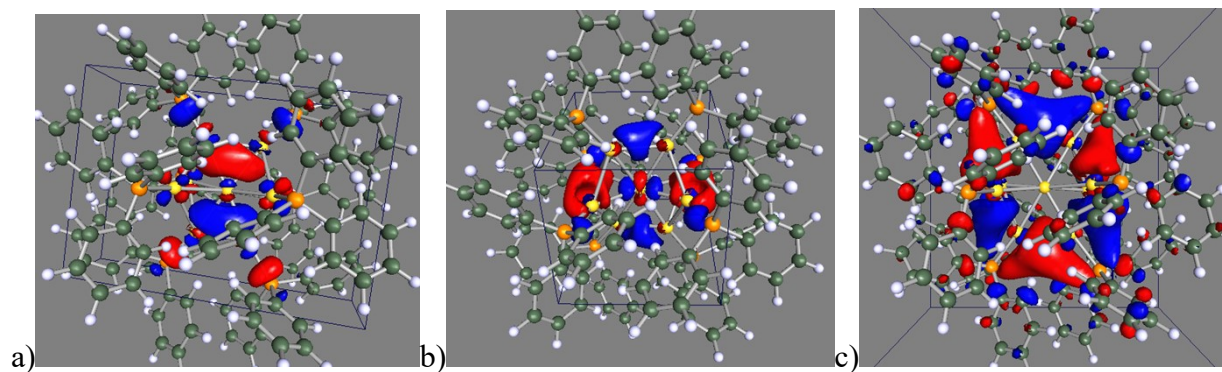
Figure S15. Key orbitals in the first TPA peak of D_2 $Au_9(PR_3)_8^{3+}$ with R = Ph. a) HOMO with superatom P character. b) LUMO with superatom D character. c) LUMO+3 with superatom F character.

Coordinates optimized at the PBE0-D3 level of theory.

Au$_8$(PR$_3$)$_7{}^{2+}$, R=Ph

Au	0.02350300	0.03033800	-0.24326999
Au	-2.12389493	-1.53341806	-0.20300101
Au	0.21807501	-2.33780408	1.32655203
Au	-2.34067392	1.21515405	-0.68926197
Au	0.50079697	-2.44351792	-1.32364094
Au	2.55168295	-0.77397001	0.19072101
Au	1.99777305	1.71778095	-0.83749199
Au	-0.23360300	2.39173388	0.86705899
P	-3.87126899	-3.03681207	-0.07480800
P	0.12862700	-2.31962609	3.65413404
P	-4.24580193	2.38804007	-1.34246004
P	0.76125097	-2.24651694	-3.63901901
P	4.29350901	-2.23198104	0.66102898
P	3.46933508	3.34281206	-1.58995295
P	-0.48534200	4.10496187	2.37383699
C	-4.23438692	-3.83614898	-1.67080498
C	-4.16587496	-3.03912592	-2.82262111
C	-4.47128820	-3.58034897	-4.06752586
C	-4.83737516	-4.92277813	-4.17188215
C	-4.89488077	-5.72316313	-3.03117704
C	-4.59396601	-5.18470287	-1.78008199
C	-5.44981384	-2.31540704	0.48301801
C	-5.42987823	-1.06440496	1.11347497
C	-6.61790419	-0.46961799	1.53528595
C	-7.83332920	-1.11910999	1.32154906
C	-7.86108589	-2.36221504	0.68643701
C	-6.67453384	-2.96101189	0.26666099
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P       2.78155303      3.09612012      2.61478209
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C       4.94758177      4.04070282     -1.91003299
H       5.11442423      4.64661503     -1.01580405
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C       4.55129099      2.45780206     -4.18131685
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