Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Impact of co-adsorbed oxygen on crotonaldehyde adsorption over gold sub-nanometer particles: A computational study

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Periodic slab calculations:

The unit cell dimensions of a bulk 1x1x1 unit cell of the gold lattice were identified using PBE and 400 eV cutoff for planewave expansion. This gave a=b=c=4.200 Å which is in good agreement (within +2.9%) of the experimental lattice constant of 4.078 Å. Then a periodic slab model of the Au(111) surface was generated using these unit cell parameters. The Au-Au bond length that corresponds to these lattice vector lengths is 2.970 Å and 2.884 Å, respectively. We used the former to build a 5-layer periodic 4x4 slab with a 15 Å vacuum gap. For crotonaldehyde the coordinates of the optimized structure on Au_{13} had been used. Only the two top layer were allowed to relax during the optimization which resulted in a small reduction of the interlayer lattice spacing. For both π-bond and di-σ bond configurations, Crotonaldehyde desorbed and obtained a flat configuration, identical to the gas phase structure.

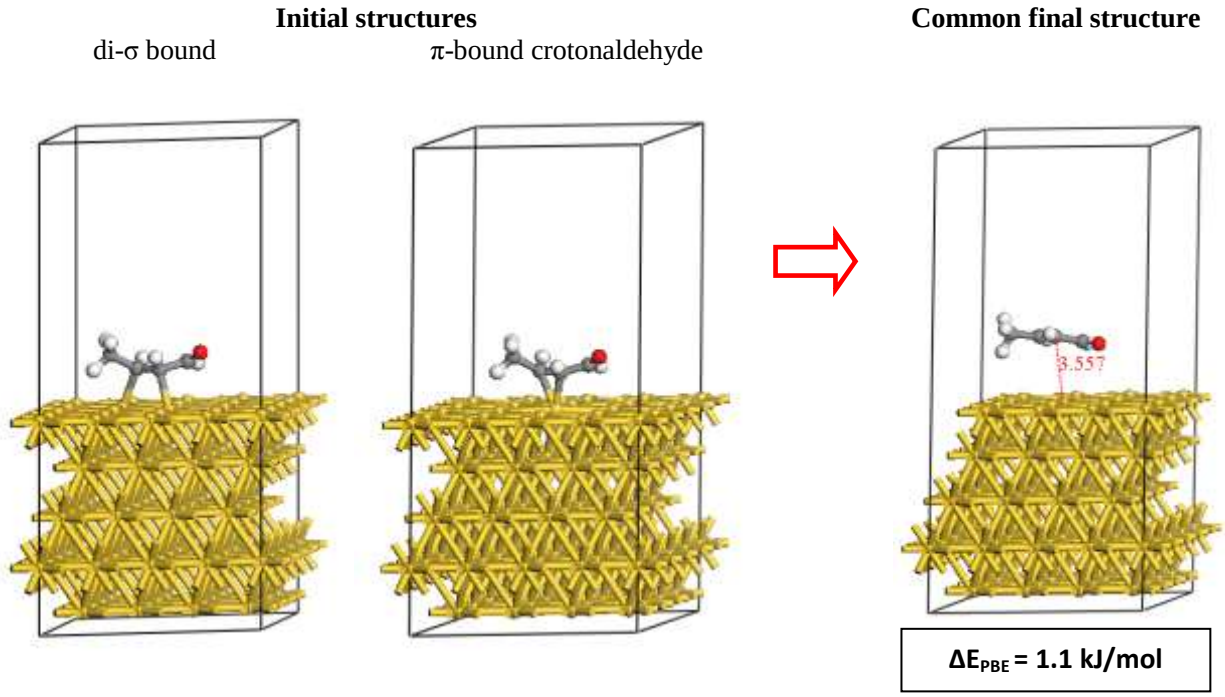

Figure S1. Optimised geometries of di-σ and π-bound crotonaldehyde over Au(111)

Cartesian coordinates of structures in Fig. 1

E-(s)-trans: B3LYP/aug-cc-pVTZ

C	-2.4218	-0.1648	0.00000
H	-2.4252	-1.2535	0.00010
H	-2.9760	0.1857	-0.87460
H	-2.9756	0.1856	0.87500
C	-1.0389	0.3887	-0.00010
H	-0.9543	1.4730	-0.00010
C	0.0910	-0.3240	-0.00010
H	0.0871	-1.4081	-0.00020
C	1.4002	0.3313	-0.00000
H	1.3652	1.4405	0.00010
O	2.4620	-0.2513	0.00010

E-(s)-trans: PBE/aug-cc-pVTZ

C	2.4285	-0.1635	0.00020
H	2.4372	-1.2605	-0.00080
H	2.9876	0.1927	0.88040
H	2.9889	0.1945	-0.87840
C	1.0455	0.3867	-0.00030
H	0.9535	1.4802	0.00040
C	-0.0933	-0.3311	-0.00040
H	-0.0891	-1.4245	-0.00040
C	-1.3997	0.3311	-0.00010
H	-1.3506	1.4521	-0.00020
O	-2.4767	-0.2468	0.00030

E-(s)-trans: PBE/Planewaves

C	11.6093	13.7853	11.3219
C	11.9741	13.3378	12.5390
C	11.9164	15.1260	10.7544
C	11.6087	11.9937	12.9867
H	11.0303	13.1035	10.6840
H	12.5514	13.9550	13.2344
H	11.0189	11.3967	12.2406
H	12.5046	15.7439	11.4458
H	12.4723	15.0294	9.8068
H	10.9864	15.6643	10.5050
O	11.9011	11.5162	14.0789

E-(s)-cis: B3LYP/aug-cc-pVTZ

C	-2.3196	-0.1177	-0.00010
H	-2.6055	0.9332	-0.00080
H	-2.7647	-0.6003	0.87430
H	-2.7644	-0.6014	-0.87400
C	-0.8426	-0.3009	0.00020
H	-0.4713	-1.3214	0.00050
C	0.0645	0.6796	0.00000
H	-0.2388	1.7211	-0.00040
C	1.5145	0.4131	0.00010
H	2.1538	1.3176	0.00040
O	2.0238	-0.6866	-0.00020

E-(s)-cis: PBE/aug-cc-pVTZ

C	-2.3237	-0.1193	0.00010
H	-2.6158	0.9386	0.00020
H	-2.7730	-0.6097	0.87900
H	-2.7735	-0.6099	-0.87830
C	-0.8478	-0.3010	-0.00030
H	-0.4672	-1.3286	-0.00020
C	0.0667	0.6865	-0.00010
H	-0.2406	1.7367	0.00010
C	1.5173	0.4167	-0.00000
H	2.1635	1.3303	0.00020
O	2.0289	-0.6944	0.00010

E-(s)-cis: PBE/Planewaves

C	11.6043	13.7893	11.3081
C	11.9645	13.3327	12.5229
C	11.9212	15.1332	10.7574
C	11.6076	11.9828	12.9948
H	11.0259	13.1070	10.6730
H	12.5424	13.9602	13.2100
H	11.9660	11.7333	14.0261
H	12.5071	15.7455	11.4564
H	12.4817	15.0416	9.8116
H	10.9942	15.6755	10.5040
O	10.9690	11.1543	12.3513

Z-(s)-trans: B3LYP/aug-cc-pVTZ

C	2.0043	-0.6034	0.00000
H	1.4259	-1.5229	-0.00010
H	2.6602	-0.6110	0.87440
H	2.6603	-0.6109	-0.87420
C	1.1711	0.6370	-0.00000
H	1.7410	1.5615	0.00010
C	-0.1637	0.7497	-0.00010
H	-0.6200	1.7324	-0.00000
C	-1.1155	-0.3634	-0.00010
H	-0.6920	-1.3840	-0.00020
O	-2.3192	-0.2105	0.00010

Z-(s)-trans: PBE/aug-cc-pVTZ

C	-2.0075	-0.6057	0.00010
H	-1.4217	-1.5306	0.00050
H	-2.6719	-0.6158	-0.87850
H	-2.6710	-0.6151	0.87960
C	-1.1801	0.6375	-0.00030
H	-1.7559	1.5694	-0.00030
C	0.1653	0.7524	0.00010
H	0.6236	1.7442	0.00060
C	1.1159	-0.3617	-0.00030
H	0.6821	-1.3912	-0.00080
O	2.3316	-0.2120	0.00020

Z-(s)-trans: PBE/Planewaves

C	11.6014	13.7479	11.3018
C	11.9439	13.2905	12.5262
C	10.8332	13.0485	10.2299
C	11.6178	11.9694	13.0638
H	11.9224	14.7647	11.0451
H	12.5148	13.9315	13.2042
H	11.0343	11.2835	12.4012
H	10.5125	12.0357	10.4991
H	9.9392	13.6364	9.9624
H	11.4396	12.9878	9.3106
O	11.9525	11.5953	14.1866

Z-(s)-cis: B3LYP/aug-cc-pVTZ

C	1.6209	-0.7562	0.00010
H	0.8298	-1.4972	0.00020
H	2.2620	-0.9089	0.87330
H	2.2620	-0.9092	-0.87310
C	1.1004	0.6399	-0.00010
H	1.8608	1.4161	-0.00020
C	-0.1750	1.0546	-0.00010
H	-0.3697	2.1211	-0.00020
C	-1.3863	0.2176	0.00020
H	-2.3290	0.8010	0.00070
O	-1.4345	-0.9948	-0.00020

Z-(s)-cis: PBE/aug-cc-pVTZ

C	1.6181	-0.7600	0.00000
H	0.8131	-1.4994	-0.00040
H	2.2658	-0.9202	0.87790
H	2.2666	-0.9201	-0.87730
C	1.1094	0.6392	-0.00010

H	1.8787	1.4198	-0.00010
C	-0.1751	1.0596	0.00000
H	-0.3685	2.1357	0.00000
C	-1.3876	0.2234	0.00000
H	-2.3385	0.8155	0.00010
O	-1.4383	-1.0006	-0.00000

Z-(s)-cis: PBE/Planewaves

C	11.5914	13.7506	11.2938
C	11.9358	13.2773	12.5132
C	10.8250	13.0578	10.2226
C	11.6285	11.9525	13.0746
H	11.9134	14.7726	11.0573
H	12.5035	13.9314	13.1827
H	12.0050	11.8081	14.1207
H	10.4927	12.0592	10.5224
H	9.9550	13.6703	9.9296
H	11.4476	12.9777	9.3141
O	11.0239	11.0373	12.5181

Cartesian coordinates of structures in Fig. 2

Au_{13}

Au	10.4181	10.4777	11.9614
Au	12.4234	10.4777	9.9561
Au	14.4288	10.4777	11.9614
Au	10.4181	12.4830	9.9561
Au	10.4181	14.4884	11.9614
Au	12.4234	12.4830	11.9614
Au	12.4234	14.4884	9.9561
Au	14.4288	12.4830	9.9561
Au	14.4288	14.4884	11.9614
Au	12.4234	10.4777	13.9668
Au	10.4181	12.4830	13.9668
Au	12.4234	14.4884	13.9668
Au	14.4288	12.4830	13.9668

$Au_{13}O_2$ (1)

Au	13.7223	11.8591	15.9647
Au	14.6990	9.9900	14.1305
Au	12.3656	9.6233	12.6192
Au	11.3243	11.7697	14.5092
Au	16.0547	12.3929	14.6151
Au	14.8369	14.8476	13.4831
Au	15.8860	12.7008	11.5872
Au	13.6049	12.2349	13.0479
Au	14.7333	10.1381	11.3415
Au	13.4931	12.6182	10.1327
Au	12.4735	14.3324	14.7642
Au	12.5049	14.4793	11.9730
Au	11.1579	12.0753	11.4744
O	10.4485	10.6133	12.9245
O	16.7564	13.8677	13.1706

$Au_{13}O_2$ (2)

Au	13.6395	11.8318	15.8057
Au	14.7732	9.7755	14.2155
Au	12.3461	9.7738	12.7443
Au	11.1409	11.7048	14.4556
Au	16.0303	12.2214	14.4133
Au	14.7767	14.7782	13.2262
Au	16.2242	12.8357	11.5227
Au	13.5859	12.2514	13.0440
Au	14.8043	10.2490	11.5041
Au	13.5162	12.7801	10.2990
Au	12.4767	14.2108	14.7016
Au	12.3520	14.6991	11.9117
Au	11.1584	12.1431	11.6459
O	15.3801	11.6998	9.9830
O	16.7702	13.9000	13.2391

$Au_{13}O_4$ (1)

Au	13.4906	12.0195	15.7781
Au	14.8773	9.8566	14.0564
Au	12.5047	9.7426	12.7023
Au	11.1007	11.8649	14.4573
Au	16.2102	12.3671	14.3714
Au	15.0205	14.5930	13.3379
Au	16.1403	12.7040	11.7079
Au	13.6000	12.2510	13.0343
Au	14.8562	10.1679	11.3891
Au	13.3816	12.6460	10.3145
Au	12.3032	14.2490	14.7494
Au	12.2783	14.5737	11.9091
Au	11.0269	12.2148	11.6197
O	10.5231	10.4653	12.8633

O	15.3437	11.0022	15.8727
O	13.2646	15.7661	13.4689
O	15.2646	11.7642	9.9235

$Au_{13}O_4$ (2)

Au	13.7297	11.8017	15.6506
Au	14.9270	9.8667	14.0393
Au	12.4365	9.7522	12.9773
Au	10.9852	11.7466	14.5310
Au	16.2345	12.4773	14.4420
Au	14.9343	14.6469	13.4494
Au	16.1088	12.7807	11.7271
Au	13.5640	12.2907	12.9911
Au	14.6218	10.1901	11.3010
Au	13.4781	12.6534	10.2362
Au	12.4110	14.4864	14.7951
Au	12.2863	14.5254	11.8201
Au	11.1196	12.1042	11.4478
O	10.4333	10.6085	12.9234
O	11.8233	12.9296	15.9999
O	13.1198	15.8235	13.3886
O	15.4480	11.7135	9.9930

$Au_{13}O_4$ (3)

Au	13.8440	12.0446	15.7586
Au	14.7401	9.7657	14.2731
Au	12.4530	9.8068	12.5723
Au	11.0328	11.6456	14.5746
Au	16.1718	12.0741	14.3056
Au	14.7440	14.6928	13.5369
Au	16.1753	12.8699	11.5134
Au	13.6014	12.2533	13.0377
Au	14.9941	10.2085	11.6025
Au	13.3776	12.4908	10.3148
Au	12.1935	14.3044	14.4719
Au	12.4638	14.7426	11.8047
Au	11.0444	12.4239	11.7675
O	10.4627	10.5956	12.8936
O	11.8436	12.8035	16.0759
O	15.3741	11.7120	10.0070
O	16.7354	13.9194	13.1980

$Au_{13}O_4$ (4)

Au	13.5757	11.8533	15.9770
Au	14.9289	9.9911	13.8248
Au	12.4786	9.8138	12.4365
Au	11.0976	11.6853	14.5489
Au	16.0703	12.5576	14.5620
Au	15.0492	14.7374	13.2575
Au	15.9427	12.5836	11.8137
Au	13.4961	12.3633	13.1836
Au	14.8369	9.9459	11.1371
Au	13.4453	12.4411	10.3844
Au	12.4543	14.5296	14.7594
Au	12.3851	14.5637	11.7811
Au	11.0166	12.1983	11.6377
O	10.5269	10.4577	13.0100
O	11.8191	12.9908	16.0169
O	13.1736	15.8649	13.3717
O	15.3142	10.7870	15.7669

$Au_{13}O_4$ (5)

Au	13.6195	11.8682	16.0429
Au	14.6728	9.9099	14.0310
Au	12.3586	9.9589	12.4994
Au	11.1822	11.7478	14.2689
Au	16.2580	12.4176	14.5810

Au	15.0076	14.9160	13.3230
Au	15.9175	12.6394	11.5927
Au	13.6827	12.3782	13.2247
Au	14.8744	10.0946	11.2752
Au	13.4390	12.3292	10.3839
Au	12.4045	14.4240	14.8675
Au	12.4119	14.4445	11.8634
Au	10.8961	12.1530	11.5488
O	15.4637	10.9457	15.8112
O	11.7932	12.8497	16.0782
O	13.1272	15.7783	13.4677
O	16.7960	13.8712	13.1975

$Au_{13}O_6$ (1)

Au	13.6276	11.8504	15.8771
Au	14.6896	9.9343	14.2697
Au	12.3398	9.5008	12.6813
Au	11.0173	11.7164	14.5736
Au	15.9548	12.2828	14.6164
Au	15.0948	14.8604	13.2881
Au	16.1735	12.8543	11.5782
Au	13.5899	12.2389	13.0478
Au	14.9086	10.2783	11.1502
Au	13.3412	12.5890	10.2468
Au	12.5099	14.5100	14.7466
Au	12.3022	14.4643	11.8816
Au	11.1004	12.0625	11.6255
O	10.5537	10.4241	13.0525
O	11.7479	13.0504	15.9586
O	13.2875	15.8107	13.3266
O	15.4021	11.8950	9.9445
O	16.8516	13.7706	13.2886
O	14.2689	8.8019	12.4108

$Au_{13}O_6$ (2)

Au	13.5251	11.8856	15.9810
Au	14.8111	9.8573	13.8891
Au	12.4606	9.6994	12.5944
Au	11.0944	11.7117	14.5946
Au	16.1463	12.2501	14.7026
Au	15.0505	14.8316	13.2860
Au	16.1622	12.8806	11.6048
Au	13.6336	12.3056	13.1129
Au	14.6870	10.2618	11.2188
Au	13.3455	12.5595	10.2336
Au	12.4817	14.5507	14.6865
Au	12.2431	14.4112	11.8415
Au	11.1040	11.9730	11.5759
O	10.4945	10.4639	13.1214
O	15.2413	10.7754	15.8536
O	11.8233	13.0870	15.9821
O	13.2528	15.8102	13.2240
O	15.4200	11.9691	9.9594
O	16.8042	13.7132	13.4057

$Au_{13}O_8$

Au	13.4068	12.0010	16.0505
Au	14.8722	9.8616	14.3091
Au	12.4734	9.4574	12.7077
Au	11.0237	11.6342	14.4186
Au	16.1509	12.3515	14.6021
Au	15.2214	14.8043	13.3322
Au	16.1033	12.7436	11.4732
Au	13.6052	12.2528	13.0388
Au	14.8247	10.2533	11.1807
Au	13.3139	12.7476	10.0651
Au	12.4600	14.4278	14.7429

Au	12.4164	14.7740	11.9545
Au	10.9792	11.9805	11.6308
O	10.6119	10.3335	12.8478
O	15.2424	11.0668	15.9634
O	11.5670	12.9678	15.9014
O	13.4118	15.7798	13.4796
O	15.1499	11.8314	9.8649
O	16.9225	13.6149	13.1595
O	14.4445	8.7917	12.5925
O	11.4812	13.6378	10.5026

Cartesian coordinates of structures in Fig. 3

Au_{13}-crotonaldehyde-di-σ-1

Au	13.747287194	12.269866118	15.9524
Au	15.112569314	10.139509536	14.6681
Au	12.705896853	9.477574304	13.4085
Au	11.253410575	11.656342281	14.5947
Au	16.112005524	12.765075786	14.3090
Au	14.693763023	14.762339233	13.0086
Au	15.845273793	12.686988949	11.4409
Au	13.633492934	12.160319667	13.1555
Au	14.927382644	9.980489347	11.8543
Au	13.487312747	11.823961825	10.2889
Au	12.440536833	14.282541490	14.5561
Au	12.264591503	14.186497362	11.7138
Au	11.213737577	11.283365120	11.8622
O	9.238849600	8.860413818	10.1731
C	12.070873160	10.748600216	9.0063
C	10.848700133	10.592444673	9.7938
C	11.984128895	11.552623192	7.7228
C	10.413962228	9.214155999	10.1479
H	12.643297136	9.814012719	8.9079
H	10.017169561	11.256307368	9.5117
H	11.245008782	8.489816265	10.3442
H	11.492890346	12.524413042	7.8749
H	12.971166401	11.724122373	7.2730
H	11.377935418	10.988363518	6.9890

Au_{13}-crotonaldehyde-di-σ-2

Au	13.7293	12.2754	15.9415
Au	15.1370	10.1636	14.6887
Au	12.7257	9.4788	13.4097
Au	11.2594	11.6809	14.5927
Au	16.1192	12.8008	14.3448
Au	14.6957	14.7794	13.0253
Au	15.8621	12.6507	11.4581
Au	13.6581	12.1617	13.1489
Au	14.9706	9.9526	11.8917
Au	13.5150	11.7515	10.3170
Au	12.4275	14.2786	14.5381
Au	12.2561	14.1732	11.7241
Au	11.2090	11.2693	11.8672
O	12.5763	11.7185	6.9690
C	12.0025	10.7218	9.0741
C	10.7935	10.4935	9.8630
C	11.9678	11.7850	8.0334
C	10.2990	9.0677	9.9884
H	12.5614	9.8256	8.7749
H	9.9994	11.2305	9.6536
H	11.0994	8.3901	10.3162
H	11.2862	12.6447	8.2584
H	9.9479	8.7155	9.0010
H	9.4603	8.9820	10.6913

Au_{13}-crotonaldehyde-π-bonded

Au	13.2236	11.6409	16.0339
Au	14.2799	9.5657	14.4446
Au	11.9241	9.5300	12.9406
Au	10.8635	11.5946	14.5159
Au	15.6556	11.9918	14.6926
Au	14.8951	14.4264	13.5197
Au	15.9281	12.3593	11.9142
Au	13.3225	12.0024	13.1557
Au	14.4546	9.9638	11.6420
Au	13.5646	12.4147	10.3719
Au	12.3213	14.0385	14.7523
Au	12.5916	14.5258	11.9671

Au	11.0277	12.0939	11.6655
O	7.2472	11.3137	12.5908
C	9.5944	12.0222	9.9239
C	8.8509	12.2363	11.0945
C	9.8278	13.0541	8.8645
C	8.1622	11.1294	11.7990
H	9.7227	10.9776	9.6082
H	8.5023	13.2435	11.3470
H	8.5065	10.0994	11.5288
H	9.7547	14.0766	9.2557
H	10.8090	12.9252	8.3879
H	9.0634	12.9266	8.0768

Au_{13}-crotonaldehyde-atop

Au	10.5666	10.4499	10.0471
Au	8.3633	12.1697	10.0130
Au	10.0478	14.4345	10.1638
Au	12.2784	12.6917	10.1168
Au	8.5687	10.2475	12.0918
Au	10.5543	10.3160	14.1687
Au	12.4355	10.7219	12.1282
Au	8.3490	12.0288	14.2919
Au	8.0743	13.9962	12.2193
Au	10.2655	12.4316	12.1742
Au	10.0504	14.2929	14.3188
Au	12.2714	12.5533	14.2621
Au	12.0449	14.5342	12.2529
O	6.0152	14.8828	12.3987
C	4.9404	12.8102	11.8674
C	3.7684	12.1390	11.7912
C	4.9827	14.1890	12.2736
C	3.6237	10.7247	11.3730
H	2.8480	12.6736	12.0606
H	5.8961	12.3303	11.6149
H	4.0145	14.6859	12.4937
H	2.9317	10.6478	10.5164
H	4.5849	10.2711	11.1007
H	3.1618	10.1308	12.1801

$Au_{13}O_8$-crotonaldehyde-di-σ-1

Au	13.690992936	12.242228637	16.1636
Au	15.175410545	10.081137521	14.7374
Au	12.585108831	9.344599210	13.2917
Au	11.108121205	11.571653426	14.6146
Au	16.284347101	12.771716027	14.4538
Au	14.951160115	14.899372087	13.0822
Au	16.000203185	12.633507058	11.3445
Au	13.698507565	12.144871850	13.2141
Au	14.965783544	9.909656188	11.6443
Au	13.414934938	12.128287592	10.1398
Au	12.372257263	14.368217803	14.7903
Au	12.280615252	14.458358080	11.8869
Au	11.021699302	11.545990713	11.7687
O	10.643158191	10.118968579	13.2005
O	15.661923681	11.617178193	16.0618
O	11.701627183	12.884007467	16.0832
O	13.059507241	15.695932642	13.3531
O	15.246776748	11.207056101	10.0180
O	16.756730011	13.913331549	12.7718
O	9.346309764	8.757141923	9.9742
O	14.560040816	8.720336680	13.2911
O	11.596808278	13.128152336	10.4914
C	12.078205889	10.814503072	9.0307
C	10.819491457	10.630440561	9.8064
C	11.912947261	11.411555055	7.6515
C	10.470898631	9.204186405	10.1277
H	12.725249599	9.925146549	9.0579
H	9.958558561	11.189327783	9.4167

H	11.315863817	8.568601695	10.4909
H	11.392466675	12.378169761	7.6901
H	12.876170710	11.534734117	7.1392
H	11.295937983	10.726741066	7.0402

$Au_{13}O_8$-crotonaldehyde-di-σ-2

Au	13.4414	11.8180	16.0016
Au	14.8963	9.7852	14.2373
Au	12.4388	9.5489	12.6671
Au	11.0183	11.6768	14.4956
Au	16.1639	12.3199	14.6179
Au	15.1476	14.8233	13.3934
Au	16.1309	12.7843	11.5042
Au	13.6723	12.2825	13.0356
Au	14.8615	10.2471	11.1356
Au	13.3729	12.6844	10.0742
Au	12.4780	14.3756	14.8459
Au	12.4423	14.7883	11.9180
Au	10.9598	12.1052	11.5692
O	7.5602	11.8177	15.5795
O	10.6078	10.4506	12.8282
O	15.2983	10.9357	15.9221
O	14.3545	8.7809	12.5076
O	11.6486	12.8740	16.0415
O	13.2948	15.7564	13.5385
O	11.5597	13.6673	10.3792
O	15.2439	11.8469	9.8634
O	16.8781	13.6732	13.2219
C	9.0232	12.6548	12.4259
C	9.1104	12.5348	13.9054
C	8.6535	14.0237	11.9077
C	8.1684	11.5604	14.5512
H	8.4597	11.8313	11.9640
H	9.1539	13.4946	14.4392
H	8.0392	10.5914	14.0116
H	9.3346	14.8022	12.2818
H	8.6438	14.0595	10.8111
H	7.6377	14.2735	12.2663

$Au_{13}O_8$-crotonaldehyde-π-bonded

Au	13.4977	11.9015	16.3303
Au	14.8497	9.7237	14.6216
Au	12.4128	9.5016	12.8995
Au	11.0957	11.6617	14.6472
Au	16.2250	12.2078	14.8721
Au	15.3472	14.6636	13.6049
Au	16.3184	12.5230	11.7629
Au	13.6511	12.1406	13.2478
Au	14.9246	10.0455	11.5088
Au	13.6820	12.5713	10.2749
Au	12.5960	14.3273	15.0170
Au	12.6439	14.6894	12.1633
Au	11.0988	11.9890	11.6059
O	10.5923	10.4448	13.0333
O	15.3170	10.9393	16.2414
O	11.6696	12.8911	16.1926
O	13.5432	15.6684	13.7465
O	15.4457	11.5298	10.1489
O	17.0400	13.4691	13.4480
O	7.3440	12.2632	12.7589
O	14.3098	8.6642	12.9245
O	11.9541	13.6677	10.5260
C	9.5036	11.9845	9.8893
C	8.9822	12.5395	11.0616
C	9.8988	12.7418	8.6719
C	8.1101	11.7389	11.9659
H	9.3695	10.9010	9.7632
H	8.9176	13.6272	11.1749

H	8.1757	10.6314	11.8472
H	10.1033	13.7980	8.8781
H	10.7736	12.2920	8.1813
H	9.0625	12.6689	7.9522

Au_{38}-crotonaldehyde-di-σ-1

Au	14.0783	11.1112	10.4857
Au	11.7499	9.5435	10.0930
Au	11.7314	11.4415	12.1300
Au	9.5297	11.2760	10.2676
Au	15.6266	13.4915	10.0804
Au	13.6478	13.4934	12.0276
Au	13.7253	15.6840	10.1660
Au	11.6374	13.4230	10.0767
Au	11.6351	15.5106	11.9858
Au	9.6814	13.4497	12.0982
Au	9.3893	15.6958	10.3316
Au	7.6720	13.4143	10.0940
Au	11.6176	17.6933	10.1397
Au	15.5838	11.5263	8.1186
Au	13.7026	9.4664	8.1032
Au	13.8406	11.2601	5.8965
Au	11.6773	9.4397	6.1024
Au	11.7195	11.4905	8.0500
Au	9.7032	9.5072	8.0718
Au	9.2611	11.0256	5.7153
Au	7.6447	11.3743	8.0752
Au	15.5847	13.4984	6.0688
Au	15.6230	15.5033	8.0170
Au	13.6008	13.5778	8.0821
Au	14.0069	15.8453	5.6551
Au	11.6449	13.5220	6.1207
Au	11.5167	15.5183	8.1813
Au	9.6617	13.3856	8.1004
Au	9.5127	15.6107	5.9927
Au	7.6786	13.3910	6.1179
Au	7.7186	15.4400	8.1086
Au	13.6158	17.4428	7.9850
Au	11.6739	17.4166	6.0292
Au	9.5787	17.6387	8.0492
Au	11.5982	11.4428	4.1600
Au	13.6165	13.4601	4.1045
Au	11.6367	15.4297	4.0742
Au	9.6177	13.3882	4.1341
O	8.5820	21.0140	7.5668
C	9.3862	19.4971	9.2488
C	10.4088	19.5082	10.3204
C	9.5233	20.4825	8.1537
C	9.8716	19.5997	11.7400
H	8.3491	19.3858	9.5983
H	11.2089	20.2382	10.1168
H	10.5814	20.7583	7.9030
H	10.6744	19.5613	12.4881
H	9.3288	20.5539	11.8727
H	9.1625	18.7876	11.9590

Au_{38}-crotonaldehyde-di-σ-2

Au	14.0774	11.0929	10.5137
Au	11.7299	9.5565	10.1264
Au	11.7201	11.4466	12.1621
Au	9.5020	11.2833	10.2957
Au	15.6302	13.4630	10.0970
Au	13.6584	13.4807	12.0491
Au	13.7634	15.6735	10.1843
Au	11.6510	13.3910	10.0947
Au	11.6396	15.5031	11.9583
Au	9.6698	13.4679	12.0939
Au	9.3749	15.7182	10.3441

Au	7.6293	13.4303	10.1272
Au	11.6974	17.6968	10.0831
Au	15.6028	11.4863	8.1491
Au	13.6693	9.4683	8.1351
Au	13.8289	11.2502	5.9343
Au	11.6452	9.4342	6.1311
Au	11.6818	11.4917	8.0612
Au	9.6774	9.5070	8.1087
Au	9.2441	11.0560	5.7755
Au	7.6140	11.3868	8.1253
Au	15.5930	13.4695	6.0912
Au	15.6433	15.4688	8.0371
Au	13.6132	13.5333	8.0981
Au	14.0052	15.8278	5.6974
Au	11.6185	13.5675	6.1752
Au	11.5341	15.5169	8.2421
Au	9.6348	13.4161	8.1571
Au	9.4954	15.6257	6.0536
Au	7.6537	13.4159	6.1794
Au	7.6760	15.4761	8.1451
Au	13.6748	17.4464	7.9941
Au	11.6668	17.4009	6.1028
Au	9.5335	17.6728	8.1023
Au	11.5751	11.4715	4.2207
Au	13.5962	13.4614	4.1549
Au	11.6206	15.4464	4.1153
Au	9.5889	13.4114	4.1862
O	11.0139	20.3111	12.3626
C	9.5048	19.6023	9.1351
C	10.6441	19.6480	10.0809
C	9.4831	20.6939	8.0763
C	10.3389	19.7104	11.5279
H	8.5411	19.4964	9.6576
H	11.4651	20.3177	9.7865
H	9.3949	19.1843	11.8288
H	8.6342	20.5817	7.3888
H	9.3945	21.6832	8.5629
H	10.4084	20.7058	7.4818

Au_{38}-crotonaldehyde-π-bonded

Au	10.4631	8.8158	9.4533
Au	12.8635	7.3770	9.9768
Au	12.8705	9.2230	7.9135
Au	15.1791	9.0129	9.5729
Au	9.0307	11.2089	9.8966
Au	10.9676	11.2203	7.9109
Au	10.7711	13.4569	9.6322
Au	12.9306	11.2474	9.9183
Au	12.9853	13.2541	7.8529
Au	14.9016	11.2348	7.8841
Au	15.3416	13.6109	9.4080
Au	16.8949	11.2536	9.8862
Au	13.0472	15.1587	9.8817
Au	9.1273	9.3383	11.8803
Au	10.8380	7.1465	11.8968
Au	10.6917	8.9960	14.1903
Au	12.9464	7.2920	13.8397
Au	12.4993	9.3770	11.9440
Au	14.8758	7.5539	11.8923
Au	15.3332	8.8700	14.2895
Au	17.1556	9.1881	11.8674
Au	9.0513	11.2839	13.9084
Au	8.7927	13.4187	11.9185
Au	10.9838	11.7576	11.9383
Au	10.6818	13.5753	14.3461
Au	12.9925	11.2990	13.9064
Au	13.4512	13.1843	11.8975
Au	14.8934	10.8180	11.8720

Au	15.1968	13.4168	14.2426
Au	16.8759	11.1892	13.8417
Au	16.5884	13.1807	11.8642
Au	11.1576	14.9592	11.9547
Au	13.0090	15.1603	13.9957
Au	14.9713	15.4872	11.9159
Au	12.9686	9.2574	15.8336
Au	10.9674	11.2449	15.9369
Au	13.0054	13.1772	16.0085
Au	15.0210	11.1428	15.9656
O	7.4478	16.9696	13.0063
C	6.4919	13.6212	12.0209
C	7.0400	14.9008	11.8942
C	5.7968	12.8824	10.9225
C	7.2647	15.7611	13.0771
H	6.3020	13.2614	13.0401
H	7.0559	15.4062	10.9230
H	7.2206	15.2335	14.0642
H	6.0785	13.2540	9.9281
H	5.9964	11.8016	10.9704
H	4.7055	13.0113	11.0412

Au_{38}-crotonaldehyde-atop

Au	10.3134	10.1705	9.9701
Au	12.5174	8.3719	10.1309
Au	12.5414	10.3894	8.2238
Au	14.9032	9.9967	9.7829
Au	8.4253	12.2777	10.0250
Au	10.4387	12.3592	8.1179
Au	9.8991	14.6726	9.7135
Au	12.4034	12.3941	10.1870
Au	12.3545	14.3862	8.1931
Au	14.4687	12.3924	8.2225
Au	14.4581	14.5475	10.1104
Au	16.3142	12.4208	10.3010
Au	12.2097	16.2849	10.2258
Au	8.4971	10.2716	12.1360
Au	10.3833	8.2602	12.1426
Au	9.8742	9.7078	14.6149
Au	12.3411	8.3769	14.1136
Au	12.2336	10.3792	12.1250
Au	14.3964	8.5191	12.1506
Au	14.4952	10.2215	14.3702
Au	16.4427	10.3930	12.2115
Au	8.3443	12.0468	14.2195
Au	8.1597	14.1262	12.1704
Au	10.3240	12.4378	12.1064
Au	10.0924	14.3209	14.3250
Au	12.2720	12.2572	14.1743
Au	12.4108	14.2989	12.2401
Au	14.3111	12.2709	12.2526
Au	14.6630	14.8339	14.7278
Au	16.2696	12.4410	14.2820
Au	16.1736	14.4234	12.3520
Au	10.2121	16.0740	12.1333
Au	12.2081	16.2604	14.2272
Au	14.2538	16.4122	12.3186
Au	12.2714	10.2269	16.1622
Au	10.2932	12.1549	16.1610
Au	12.2501	14.2938	16.1735
Au	14.2456	12.3810	16.1825
O	5.9417	14.8884	12.4598
C	4.8934	12.8276	11.8401
C	3.7472	12.1113	11.8273
C	4.9268	14.1737	12.3583
C	3.6172	10.7191	11.3302
H	2.8382	12.5834	12.2237
H	5.8359	12.4082	11.4693

H	3.9564	14.6033	12.6941
H	2.8339	10.6573	10.5561
H	4.5603	10.3340	10.9206
H	3.2854	10.0524	12.1451

$Au_{38}O_8$-crotonaldehyde-di-σ-1

Au	14.0550	11.1128	10.3794
Au	11.7846	9.4930	10.0948
Au	11.7920	11.3919	12.1208
Au	9.4169	11.0054	10.5330
Au	15.5859	13.5054	9.9912
Au	13.7157	13.4459	12.0228
Au	14.2274	15.8612	10.5868
Au	11.7157	13.3517	10.0845
Au	11.7354	15.4390	11.9444
Au	9.7889	13.3786	12.1046
Au	9.3370	15.7131	10.5059
Au	7.7541	13.3467	10.1755
Au	11.3738	17.6559	10.2674
Au	15.5691	11.5250	8.0214
Au	13.7096	9.4493	8.1065
Au	13.9397	11.1064	5.7516
Au	11.6443	9.3996	6.1593
Au	11.8297	11.4915	8.0037
Au	9.7722	9.4483	8.1892
Au	9.3154	10.9857	5.8967
Au	7.6774	11.2771	8.2524
Au	15.5033	13.5142	6.0613
Au	15.6342	15.5403	8.0180
Au	13.5584	13.7153	8.0784
Au	13.7367	15.7888	5.8303
Au	11.5366	13.6167	6.1716
Au	11.3437	15.5163	8.3036
Au	9.6868	13.2434	8.1775
Au	8.9650	15.7041	5.5526
Au	7.6420	13.2856	6.2805
Au	7.8744	15.3681	8.1616
Au	13.4817	17.3776	8.0571
Au	11.4809	17.3117	6.1129
Au	9.4503	17.6792	8.3572
Au	11.5714	11.4068	4.2269
Au	13.4870	13.4453	4.1543
Au	11.4655	15.3914	4.0446
Au	9.5295	13.3212	4.2528
O	9.3584	17.7368	6.1672
O	13.5465	17.8882	10.1610
O	9.3192	21.1200	7.1046
C	9.6584	19.8732	9.1110
C	10.5801	19.8457	10.1935
C	10.0787	20.4921	7.8311
C	10.0988	20.0742	11.6030
H	8.5917	19.9839	9.3523
H	11.5942	20.2054	9.9661
H	9.1580	19.5419	11.8031
H	11.1676	20.3889	7.5891
H	9.9051	21.1546	11.7384
H	10.8421	19.7813	12.3559

$Au_{38}O_8$-crotonaldehyde-di-σ-2

Au	14.0338	11.0657	10.3589
Au	11.7458	9.4872	10.0537
Au	11.7782	11.3414	12.1301
Au	9.4033	11.0065	10.5147
Au	15.5953	13.4380	10.0010
Au	13.7202	13.3863	12.0312
Au	14.2878	15.8118	10.6286
Au	11.7333	13.2736	10.0847
Au	11.7700	15.4087	11.8908

Au	9.8099	13.3640	12.1067
Au	9.3540	15.7029	10.5178
Au	7.7467	13.3501	10.2073
Au	11.4438	17.6917	10.2912
Au	15.5669	11.4837	8.0019
Au	13.6555	9.4549	8.0640
Au	13.9145	11.1250	5.7316
Au	11.6060	9.4221	6.1040
Au	11.7501	11.5001	7.9439
Au	9.7318	9.4597	8.1453
Au	9.2934	11.0444	5.8677
Au	7.6883	11.3352	8.2302
Au	15.5123	13.5022	6.0566
Au	15.6459	15.4867	8.0483
Au	13.5770	13.6377	8.0732
Au	13.7614	15.8071	5.8701
Au	11.5255	13.7082	6.1975
Au	11.4570	15.5263	8.4079
Au	9.6782	13.3460	8.2032
Au	8.9997	15.7762	5.6270
Au	7.6501	13.3548	6.2786
Au	7.7880	15.3918	8.2104
Au	13.5580	17.3864	8.1132
Au	11.5252	17.3474	6.2032
Au	9.4648	17.6319	8.4375
Au	11.5511	11.4732	4.2167
Au	13.4742	13.4952	4.1714
Au	11.4840	15.4821	4.0776
Au	9.5407	13.4131	4.2621
O	10.5872	20.2900	12.5111
O	9.4030	17.8206	6.2700
O	13.6358	17.8384	10.2236
C	9.6369	19.8800	9.0656
C	10.5428	19.8543	10.1585
C	9.9561	20.6308	7.8047
C	10.0033	19.8240	11.5385
H	8.5706	19.8165	9.3360
H	11.5163	20.3473	10.0388
H	8.9762	19.3870	11.6306
H	9.3763	20.2667	6.9457
H	9.7077	21.6976	7.9548
H	11.0257	20.5698	7.5571

$Au_{38}O_8$-crotonaldehyde-π-bonded

Au	10.5705	8.4809	9.5281
Au	12.9919	7.2580	10.1322
Au	12.8966	9.2614	8.1876
Au	15.3341	8.8656	9.5974
Au	9.1070	11.3403	9.7782
Au	11.0868	11.3864	7.8145
Au	10.6456	13.5922	9.6007
Au	12.8026	11.4342	9.9926
Au	13.0530	13.3799	8.0043
Au	14.9015	11.2458	8.1245
Au	15.3553	13.6654	9.6528
Au	16.8510	11.2806	10.0769
Au	12.9953	15.1972	10.1050
Au	9.1106	9.3448	12.0374
Au	10.8274	7.0055	12.0257
Au	10.6734	8.9286	14.2310
Au	13.0530	7.3504	13.6244
Au	12.2021	9.3989	11.7417
Au	15.1546	7.1185	11.8328
Au	15.4305	8.8024	14.1029
Au	17.0845	9.1194	11.7965
Au	9.0660	11.2352	14.0449
Au	8.6336	13.4632	11.7279
Au	10.8299	11.8599	11.9962

Au	10.6979	13.8280	14.6527
Au	12.8593	11.1134	13.8238
Au	13.4031	13.1659	12.0551
Au	14.7534	10.6899	11.8620
Au	15.4909	13.5654	14.2146
Au	16.9650	11.2406	13.5984
Au	17.0112	13.3550	11.8914
Au	11.0482	14.8720	12.0656
Au	13.0823	15.1522	13.9802
Au	15.0984	15.3856	11.9945
Au	13.1112	9.1315	15.7695
Au	11.1379	11.1514	15.9759
Au	13.1549	13.0905	15.8112
Au	15.1002	11.1281	15.6356
O	7.4457	17.0589	12.7007
O	8.6970	13.2549	14.4194
O	8.6019	9.2599	9.9183
C	6.3573	13.6936	11.9416
C	6.9028	14.9587	11.7193
C	5.6004	12.9055	10.9209
C	7.2298	15.8616	12.8531
H	6.2530	13.3772	12.9900
H	6.8622	15.4200	10.7275
H	7.2460	15.3767	13.8576
H	5.8286	13.2281	9.8965
H	5.7994	11.8275	11.0096
H	4.5188	13.0444	11.0950

Cartesian coordinates of structures in Fig. 4

Au_{13}-crotonaldehyde-di-σ-2

Au	13.7293	12.2754	15.9415
Au	15.1370	10.1636	14.6887
Au	12.7257	9.4788	13.4097
Au	11.2594	11.6809	14.5927
Au	16.1192	12.8008	14.3448
Au	14.6957	14.7794	13.0253
Au	15.8621	12.6507	11.4581
Au	13.6581	12.1617	13.1489
Au	14.9706	9.9526	11.8917
Au	13.5150	11.7515	10.3170
Au	12.4275	14.2786	14.5381
Au	12.2561	14.1732	11.7241
Au	11.2090	11.2693	11.8672
O	12.5763	11.7185	6.9690
C	12.0025	10.7218	9.0741
C	10.7935	10.4935	9.8630
C	11.9678	11.7850	8.0334
C	10.2990	9.0677	9.9884
H	12.5614	9.8256	8.7749
H	9.9994	11.2305	9.6536
H	11.0994	8.3901	10.3162
H	11.2862	12.6447	8.2584
H	9.9479	8.7155	9.0010
H	9.4603	8.9820	10.6913

$Au_{13}O_2$-crotonaldehyde-di-σ-2

Au	13.4721	11.9827	15.8785
Au	14.5673	9.8961	14.1429
Au	12.3442	9.7498	12.5178
Au	11.0878	12.2613	14.5646
Au	16.0947	12.3273	14.5512
Au	15.1929	14.6681	13.4183
Au	16.0297	12.6156	11.7632
Au	13.5923	12.2672	13.1314
Au	14.7879	10.1757	11.3047
Au	13.4579	12.5158	10.3658
Au	12.6788	14.4667	14.8617
Au	12.5266	14.5698	11.9172
Au	10.9936	12.3252	11.6163
O	7.8216	11.4945	15.7083
O	10.4801	10.3026	12.0061
O	13.4240	15.9042	13.4343
C	8.9555	12.7060	12.5264
C	9.0213	12.6317	13.9771
C	8.5475	14.0106	11.8951
C	8.4012	11.4374	14.6286
H	8.5633	11.7975	12.0498
H	8.8286	13.5737	14.5104
H	8.4643	10.4919	14.0386
H	9.1167	14.8606	12.2976
H	8.6458	13.9985	10.8017
H	7.4801	14.1892	12.1287

$Au_{13}O_4$-crotonaldehyde-di-σ-2

Au	14.0889	11.7924	15.7042
Au	15.4434	10.0318	14.0598
Au	13.0145	9.5503	12.8581
Au	11.4022	11.4239	14.4433
Au	16.4883	12.5925	14.5675
Au	15.1548	14.6104	13.2177
Au	16.4141	12.6190	11.7610
Au	13.8112	12.1996	12.9765
Au	15.2229	10.1276	11.2610
Au	14.1211	12.4671	10.2382

Au	12.5788	14.2323	14.7183
Au	12.5791	14.5251	11.6713
Au	11.3959	11.7176	11.3956
O	7.6633	11.2536	15.7718
O	10.9249	10.2604	12.7861
O	12.0814	12.6559	15.9655
O	13.1987	15.6249	13.3119
O	12.0478	13.2289	10.1388
C	7.9805	13.0995	12.7187
C	7.9805	12.8736	14.0483
C	8.2289	14.4057	12.0541
C	7.7121	11.5380	14.5772
H	7.7822	12.2438	12.0595
H	8.1718	13.6708	14.7728
H	7.5440	10.7479	13.8002
H	8.4418	15.2062	12.7750
H	9.0769	14.3247	11.3523
H	7.3592	14.7002	11.4425

$Au_{13}O_6$-crotonaldehyde-di-σ-2

Au	13.4454	11.8335	16.0374
Au	14.9376	9.8084	14.2314
Au	12.4516	9.5082	12.6593
Au	11.0310	11.6709	14.4755
Au	16.1824	12.3435	14.5706
Au	14.9522	14.7773	13.3653
Au	15.8719	12.7881	11.5038
Au	13.6055	12.1844	13.1535
Au	14.7207	10.4096	11.1256
Au	13.4657	12.5736	10.2284
Au	12.6283	14.3534	14.7079
Au	12.6128	14.7274	12.0317
Au	10.9658	12.1617	11.5304
O	7.5582	11.8302	15.5489
O	10.6414	10.4821	12.7766
O	15.3271	10.9868	15.9072
O	14.3684	8.7516	12.5638
O	11.6230	12.8151	16.0570
O	11.5754	13.6961	10.3490
O	16.8828	13.6852	13.2081
C	9.0461	12.6641	12.4116
C	9.1384	12.5378	13.8965
C	8.6433	14.0312	11.9089
C	8.1850	11.5668	14.5338
H	8.4820	11.8373	11.9558
H	9.1784	13.4967	14.4321
H	8.0674	10.5939	13.9986
H	9.3161	14.8178	12.2800
H	8.6246	14.0726	10.8128
H	7.6268	14.2597	12.2783

$Au_{13}O_8$-crotonaldehyde-di-σ-2

Au	13.4414	11.8180	16.0016
Au	14.8963	9.7852	14.2373
Au	12.4388	9.5489	12.6671
Au	11.0183	11.6768	14.4956
Au	16.1639	12.3199	14.6179
Au	15.1476	14.8233	13.3934
Au	16.1309	12.7843	11.5042
Au	13.6723	12.2825	13.0356
Au	14.8615	10.2471	11.1356
Au	13.3729	12.6844	10.0742
Au	12.4780	14.3756	14.8459
Au	12.4423	14.7883	11.9180
Au	10.9598	12.1052	11.5692
O	7.5602	11.8177	15.5795
O	10.6078	10.4506	12.8282
O	15.2983	10.9357	15.9221

O	14.3545	8.7809	12.5076
O	11.6486	12.8740	16.0415
O	13.2948	15.7564	13.5385
O	11.5597	13.6673	10.3792
O	15.2439	11.8469	9.8634
O	16.8781	13.6732	13.2219
C	9.0232	12.6548	12.4259
C	9.1104	12.5348	13.9054
C	8.6535	14.0237	11.9077
C	8.1684	11.5604	14.5512
H	8.4597	11.8313	11.9640
H	9.1539	13.4946	14.4392
H	8.0392	10.5914	14.0116
H	9.3346	14.8022	12.2818
H	8.6438	14.0595	10.8111
H	7.6377	14.2735	12.2663

Cartesian coordinates of structures in Fig. 5

$Au_{13}O_6$-crotonaldehyde-1

Au	13.5012	11.7857	15.9431
Au	14.9370	9.8027	13.9902
Au	12.5825	9.6928	12.7217
Au	11.0062	11.6787	14.4991
Au	16.1332	12.3696	14.4041
Au	15.1206	14.6619	13.3976
Au	16.0919	12.7558	11.7377
Au	13.5643	12.3368	13.0461
Au	14.8617	10.2053	11.3545
Au	13.4327	12.6582	10.1167
Au	12.4726	14.4135	14.8416
Au	12.4335	14.8160	11.9196
Au	10.9451	12.1001	11.5674
O	7.5477	11.8201	15.5794
O	10.5716	10.4637	12.8326
O	15.2987	10.8809	15.8575
O	11.7203	12.8600	16.0288
O	13.2305	15.8164	13.5325
O	11.6131	13.6444	10.3819
O	15.2535	11.8096	9.9075
C	9.0159	12.6542	12.4244
C	9.1031	12.5374	13.9081
C	8.6490	14.0236	11.9039
C	8.1576	11.5642	14.5513
H	8.4421	11.8335	11.9709
H	9.1414	13.4994	14.4378
H	8.0314	10.5960	14.0101
H	9.3312	14.8013	12.2772
H	8.6389	14.0576	10.8072
H	7.6332	14.2749	12.2616

$Au_{13}O_6$-crotonaldehyde-2

Au	13.4938	11.8641	15.9794
Au	14.9106	9.7446	14.1967
Au	12.4298	9.5354	12.6871
Au	11.0356	11.6733	14.5198
Au	16.1273	12.3853	14.4030
Au	15.0480	14.6417	13.3481
Au	16.1047	12.7896	11.7137
Au	13.6303	12.1623	13.0980
Au	14.8069	10.2404	11.0870
Au	13.3888	12.7810	10.2950
Au	12.4468	14.4653	14.8088
Au	12.3252	14.5962	11.9602
Au	11.0737	12.2583	11.6303
O	7.5509	11.8272	15.5160
O	10.6048	10.3755	12.9314
O	15.2757	10.8763	15.8783
O	14.3374	8.7546	12.4520
O	11.7048	12.9411	16.0166
O	13.2215	15.8355	13.4906
O	15.2580	11.8242	9.8855
C	9.0897	12.6934	12.4234
C	9.1497	12.5620	13.8977
C	8.6380	14.0377	11.9021
C	8.2051	11.5674	14.5174
H	8.5962	11.8369	11.9396
H	9.1769	13.5146	14.4450
H	8.1242	10.5911	13.9852
H	9.2522	14.8602	12.2968
H	8.6532	14.0758	10.8056
H	7.5966	14.2169	12.2300

$Au_{13}O_6$-crotonaldehyde-3

Au	13.5012	11.7857	15.9431
Au	14.9370	9.8027	13.9902
Au	12.5825	9.6928	12.7217
Au	11.0062	11.6787	14.4991
Au	16.1332	12.3696	14.4041
Au	15.1206	14.6619	13.3976
Au	16.0919	12.7558	11.7377
Au	13.5643	12.3368	13.0461
Au	14.8617	10.2053	11.3545
Au	13.4327	12.6582	10.1167
Au	12.4726	14.4135	14.8416
Au	12.4335	14.8160	11.9196
Au	10.9451	12.1001	11.5674
O	7.5477	11.8201	15.5794
O	10.5716	10.4637	12.8326
O	15.2987	10.8809	15.8575
O	11.7203	12.8600	16.0288
O	13.2305	15.8164	13.5325
O	11.6131	13.6444	10.3819
O	15.2535	11.8096	9.9075
C	9.0159	12.6542	12.4244
C	9.1031	12.5374	13.9081
C	8.6490	14.0236	11.9039
C	8.1576	11.5642	14.5513
H	8.4421	11.8335	11.9709
H	9.1414	13.4994	14.4378
H	8.0314	10.5960	14.0101
H	9.3312	14.8013	12.2772
H	8.6389	14.0576	10.8072
H	7.6332	14.2749	12.2616

$Au_{13}O_6$-crotonaldehyde-4

Au	13.4900	11.7722	15.9591
Au	14.8725	9.8003	13.9238
Au	12.4997	9.6677	12.6706
Au	10.9903	11.6485	14.5636
Au	16.1828	12.2843	14.6283
Au	15.1095	14.8392	13.3434
Au	16.1261	12.8463	11.5215
Au	13.7198	12.2915	13.1215
Au	14.7118	10.2452	11.2623
Au	13.3007	12.6721	10.2453
Au	12.4795	14.4157	14.8058
Au	12.3118	14.5122	11.9369
Au	11.0652	12.1479	11.6761
O	7.4941	11.8692	15.5080
O	10.5195	10.3707	12.9835
O	15.3024	10.8451	15.8505
O	11.7366	12.8979	16.0297
O	13.2699	15.7723	13.4559
O	15.2678	11.9122	9.9097
O	16.8570	13.7023	13.2707
C	9.0867	12.6755	12.4264
C	9.1303	12.5570	13.9054
C	8.6741	14.0226	11.8862
C	8.1535	11.5884	14.5189
H	8.5736	11.8279	11.9478
H	9.1641	13.5165	14.4407
H	8.0597	10.6104	13.9920
H	9.2889	14.8384	12.2934
H	8.7157	14.0546	10.7903
H	7.6265	14.2160	12.1875

$Au_{13}O_6$-crotonaldehyde-5

Au	13.4812	12.0371	15.8255
Au	14.8031	9.7626	14.2552
Au	12.3987	9.5614	12.6555
Au	11.1176	11.8733	14.4805

Au	16.1575	12.3861	14.4512
Au	15.0416	14.6128	13.4578
Au	16.0970	12.7616	11.7655
Au	13.6110	12.1905	12.9659
Au	14.8665	10.2094	11.1468
Au	13.4334	12.7347	10.1213
Au	12.3391	14.2361	14.7883
Au	12.4147	14.8399	11.9781
Au	10.9500	12.1036	11.5398
O	7.7280	11.7536	15.6561
O	10.5683	10.4088	12.6946
O	15.2701	10.8826	15.8815
O	14.3033	8.7483	12.5163
O	13.2250	15.8132	13.5899
O	11.6110	13.7162	10.4166
O	15.2449	11.8135	9.9059
C	9.0243	12.6704	12.4413
C	9.1414	12.5838	13.9165
C	8.6472	14.0197	11.8825
C	8.3061	11.5426	14.5975
H	8.4734	11.8254	12.0042
H	9.1069	13.5541	14.4299
H	8.2197	10.5705	14.0569
H	9.3168	14.8147	12.2423
H	8.6432	14.0303	10.7854
H	7.6265	14.2646	12.2293

$Au_{13}O_6$-crotonaldehyde-6

Au	13.3771	11.8636	15.8543
Au	14.7805	9.8244	14.0878
Au	12.4759	9.6708	12.7464
Au	11.1103	11.7300	14.3902
Au	16.1583	12.3674	14.6276
Au	15.0938	14.8236	13.4672
Au	16.1360	12.7570	11.5058
Au	13.7096	12.3198	12.9688
Au	14.7718	10.1709	11.4092
Au	13.4116	12.6377	10.1020
Au	12.3287	14.1032	14.7837
Au	12.4243	14.8000	11.9827
Au	10.9109	12.0946	11.4893
O	7.7339	11.7886	15.6537
O	10.4898	10.4111	12.6338
O	15.3075	10.9851	15.8944
O	13.2467	15.7335	13.6344
O	11.6326	13.6926	10.3983
O	15.2494	11.7541	9.9160
O	16.8445	13.7177	13.2077
C	9.0225	12.6729	12.4278
C	9.1687	12.5660	13.9059
C	8.6453	14.0369	11.9006
C	8.2939	11.5557	14.5910
H	8.4344	11.8469	12.0040
H	9.1893	13.5293	14.4317
H	8.1619	10.5911	14.0467
H	9.3351	14.8193	12.2489
H	8.6091	14.0601	10.8042
H	7.6374	14.2894	12.2785

$Au_{13}O_6$-crotonaldehyde-7

Au	13.4320	12.0007	15.8562
Au	14.7528	9.7274	14.1852
Au	12.3525	9.5718	12.6518
Au	11.1219	11.9149	14.4751
Au	16.1675	12.2544	14.6728
Au	15.0966	14.8433	13.3746
Au	16.1602	12.8247	11.5942
Au	13.7321	12.2200	13.0510

Au	14.8280	10.2457	11.1113
Au	13.3259	12.6819	10.2707
Au	12.4545	14.2678	14.7576
Au	12.3566	14.5628	11.9077
Au	11.0204	12.2521	11.6119
O	7.7797	11.6948	15.6779
O	10.5480	10.3846	12.7663
O	15.2543	10.7992	15.8570
O	14.2354	8.7507	12.4236
O	13.2976	15.8026	13.4150
O	15.3407	11.8756	9.9539
O	16.8415	13.6977	13.3515
C	9.0026	12.7068	12.4659
C	9.1060	12.6148	13.9184
C	8.6022	14.0320	11.8734
C	8.3426	11.5217	14.6042
H	8.5471	11.8258	11.9931
H	9.0697	13.5716	14.4557
H	8.2960	10.5538	14.0537
H	9.2002	14.8617	12.2775
H	8.6766	14.0376	10.7785
H	7.5449	14.2285	12.1354

$Au_{13}O_6$-crotonaldehyde-8

Au	13.5297	11.7395	15.8063
Au	14.7876	9.9418	14.3103
Au	12.4448	9.5165	12.6661
Au	11.0131	11.7126	14.5518
Au	15.9264	12.3315	14.6122
Au	14.9493	14.7710	13.4042
Au	16.1484	12.7961	11.5481
Au	13.6076	12.2231	12.9059
Au	14.8959	10.2655	11.1597
Au	13.3716	12.7128	10.0543
Au	12.6408	14.3377	14.7245
Au	12.5940	14.7385	12.0532
Au	10.9699	12.1014	11.5886
O	7.5341	11.8285	15.5612
O	10.6336	10.4699	12.8872
O	14.3547	8.7734	12.4659
O	11.6710	12.8667	16.0848
O	11.5347	13.6269	10.3572
O	15.2632	11.8818	9.8942
O	16.8846	13.6997	13.2222
C	9.0456	12.6554	12.4332
C	9.1233	12.5466	13.9204
C	8.6649	14.0201	11.9091
C	8.1750	11.5676	14.5546
H	8.4751	11.8305	11.9819
H	9.1411	13.5128	14.4439
H	8.0758	10.5907	14.0228
H	9.3407	14.8046	12.2795
H	8.6577	14.0498	10.8123
H	7.6468	14.2634	12.2653

$Au_{13}O_6$-crotonaldehyde-9

Au	13.4454	11.8335	16.0374
Au	14.9376	9.8084	14.2314
Au	12.4516	9.5082	12.6593
Au	11.0310	11.6709	14.4755
Au	16.1824	12.3435	14.5706
Au	14.9522	14.7773	13.3653
Au	15.8719	12.7881	11.5038
Au	13.6055	12.1844	13.1535
Au	14.7207	10.4096	11.1256
Au	13.4657	12.5736	10.2284
Au	12.6283	14.3534	14.7079
Au	12.6128	14.7274	12.0317

Au	10.9658	12.1617	11.5304
O	7.5582	11.8302	15.5489
O	10.6414	10.4821	12.7766
O	15.3271	10.9868	15.9072
O	14.3684	8.7516	12.5638
O	11.6230	12.8151	16.0570
O	11.5754	13.6961	10.3490
O	16.8828	13.6852	13.2081
C	9.0461	12.6641	12.4116
C	9.1384	12.5378	13.8965
C	8.6433	14.0312	11.9089
C	8.1850	11.5668	14.5338
H	8.4820	11.8373	11.9558
H	9.1784	13.4967	14.4321
H	8.0674	10.5939	13.9986
H	9.3161	14.8178	12.2800
H	8.6246	14.0726	10.8128
H	7.6268	14.2597	12.2783

$Au_{13}O_6$-crotonaldehyde-10

Au	13.5641	11.9837	15.9940
Au	14.4672	9.7529	14.2063
Au	11.8703	10.1022	12.8571
Au	11.1292	12.1503	14.5119
Au	16.2389	12.2675	14.5554
Au	15.1415	14.8173	13.3138
Au	16.2167	12.6692	11.5871
Au	13.7562	12.3571	13.0690
Au	14.4242	10.1660	11.2605
Au	13.4407	12.7213	10.1235
Au	12.8243	14.6029	14.6812
Au	12.7776	14.9164	12.0108
Au	11.0822	12.4650	11.7591
O	7.8148	11.1794	15.4635
O	15.2978	10.8522	15.7569
O	13.5873	8.8040	12.5802
O	11.9382	13.2320	16.1816
O	11.7384	13.8761	10.3091
O	15.2300	11.6614	10.0615
O	17.0199	13.6388	13.2282
C	9.0426	12.6328	12.4200
C	9.0835	12.4473	13.8828
C	8.5160	13.9460	11.8942
C	8.4530	11.1982	14.4217
H	8.6650	11.7438	11.8876
H	8.8314	13.3393	14.4753
H	8.5598	10.2889	13.7790
H	9.0298	14.8051	12.3486
H	8.6075	14.0172	10.8030
H	7.4434	14.0269	12.1520

$Au_{13}O_6$-crotonaldehyde-11

Au	13.5606	11.9350	15.8149
Au	14.4449	9.9216	14.3079
Au	11.9171	10.0964	12.8569
Au	11.1104	12.1348	14.5074
Au	16.0036	12.0707	14.5857
Au	15.4565	14.7715	13.3671
Au	16.2058	12.5818	11.5705
Au	13.6995	12.4965	12.9893
Au	14.4486	10.2025	11.2458
Au	13.4187	12.7824	10.1258
Au	12.7648	14.6805	14.8476
Au	12.6917	15.0136	11.9056
Au	11.0593	12.4338	11.7506
O	7.8328	11.1270	15.4844
O	13.6411	8.8462	12.5560
O	11.8853	13.3330	16.1228

O	13.7181	15.9089	13.4676
O	11.7265	13.9737	10.3811
O	15.1795	11.6966	9.9857
O	17.0563	13.4612	13.2396
C	9.0163	12.5917	12.4243
C	9.0583	12.4177	13.8861
C	8.4757	13.8963	11.8900
C	8.4551	11.1590	14.4332
H	8.6515	11.6946	11.8964
H	8.7957	13.3086	14.4750
H	8.5684	10.2522	13.7881
H	8.9775	14.7639	12.3421
H	8.5667	13.9656	10.7987
H	7.4018	13.9650	12.1452

$Au_{13}O_6$-crotonaldehyde-12

Au	13.5117	12.0596	16.0427
Au	14.4811	9.8084	14.2984
Au	11.8946	10.1116	12.8593
Au	11.0952	12.1432	14.5128
Au	16.2466	12.1653	14.5108
Au	15.4910	14.7510	13.3015
Au	15.9294	12.4588	11.4620
Au	13.6954	12.4757	13.1957
Au	14.3394	10.3130	11.2710
Au	13.4670	12.6397	10.3002
Au	12.7863	14.6769	14.8616
Au	12.7165	15.0408	11.9270
Au	11.0756	12.4758	11.7543
O	7.8236	11.0328	15.3937
O	15.2499	10.9384	15.8720
O	13.6210	8.8232	12.7176
O	11.8768	13.3360	16.1586
O	13.7685	15.8980	13.5002
O	11.7320	14.0271	10.4296
O	17.0670	13.4193	13.0892
C	9.0241	12.6072	12.3956
C	9.0504	12.3896	13.8532
C	8.4697	13.9173	11.8909
C	8.4640	11.1050	14.3554
H	8.6756	11.7202	11.8393
H	8.7615	13.2586	14.4627
H	8.6087	10.2189	13.6881
H	8.9489	14.7801	12.3749
H	8.5808	14.0185	10.8042
H	7.3902	13.9607	12.1273

Local-Density-of-States (LDOS) plots associated with Fig. 7

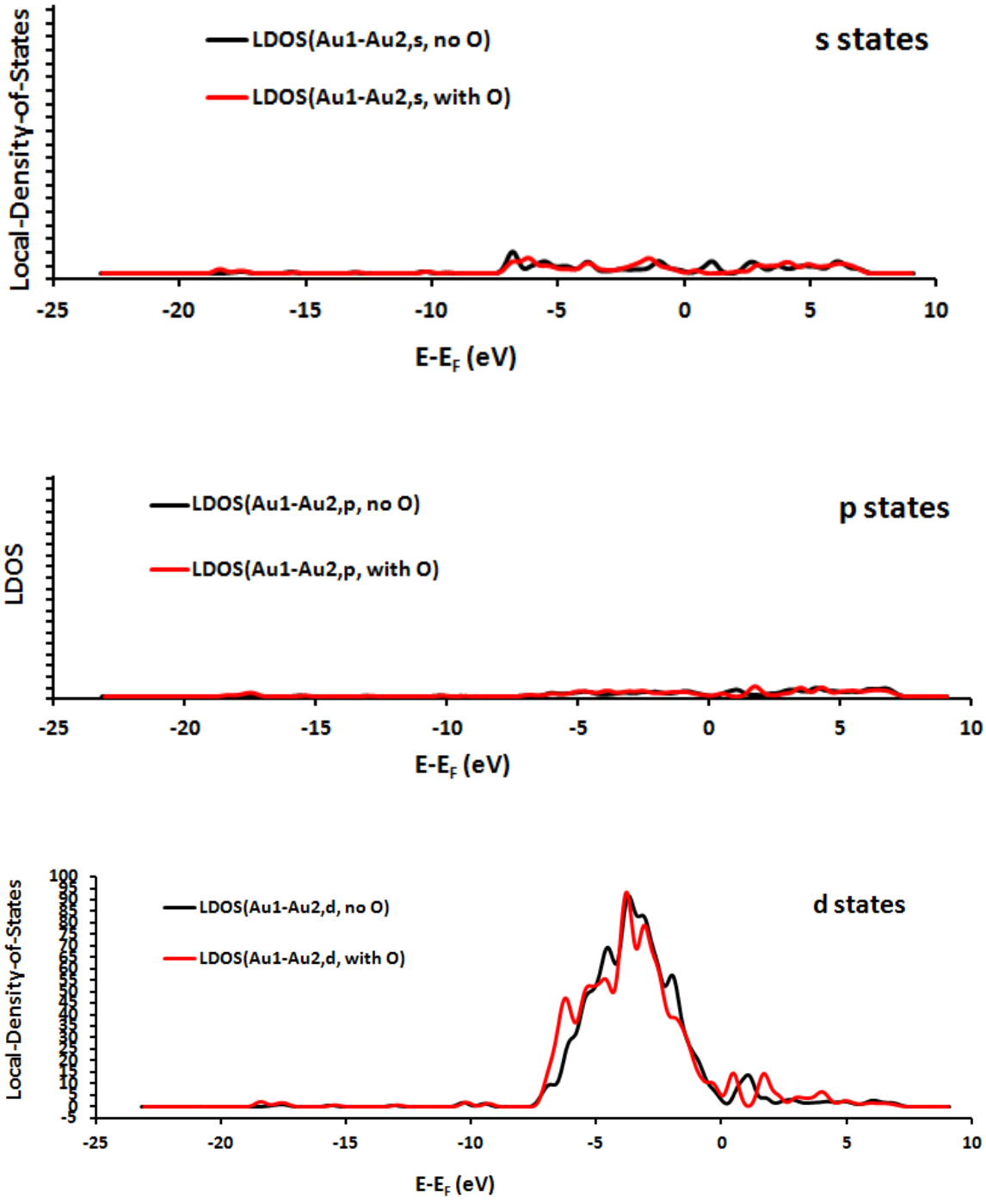

Figure S2a. LDOS plots for **E-(s)-trans-di-σ-crotonaldehyde** on $Au_{13}O_6$ (with and without neighbouring hollow O adatom) projected onto bonding gold atoms.

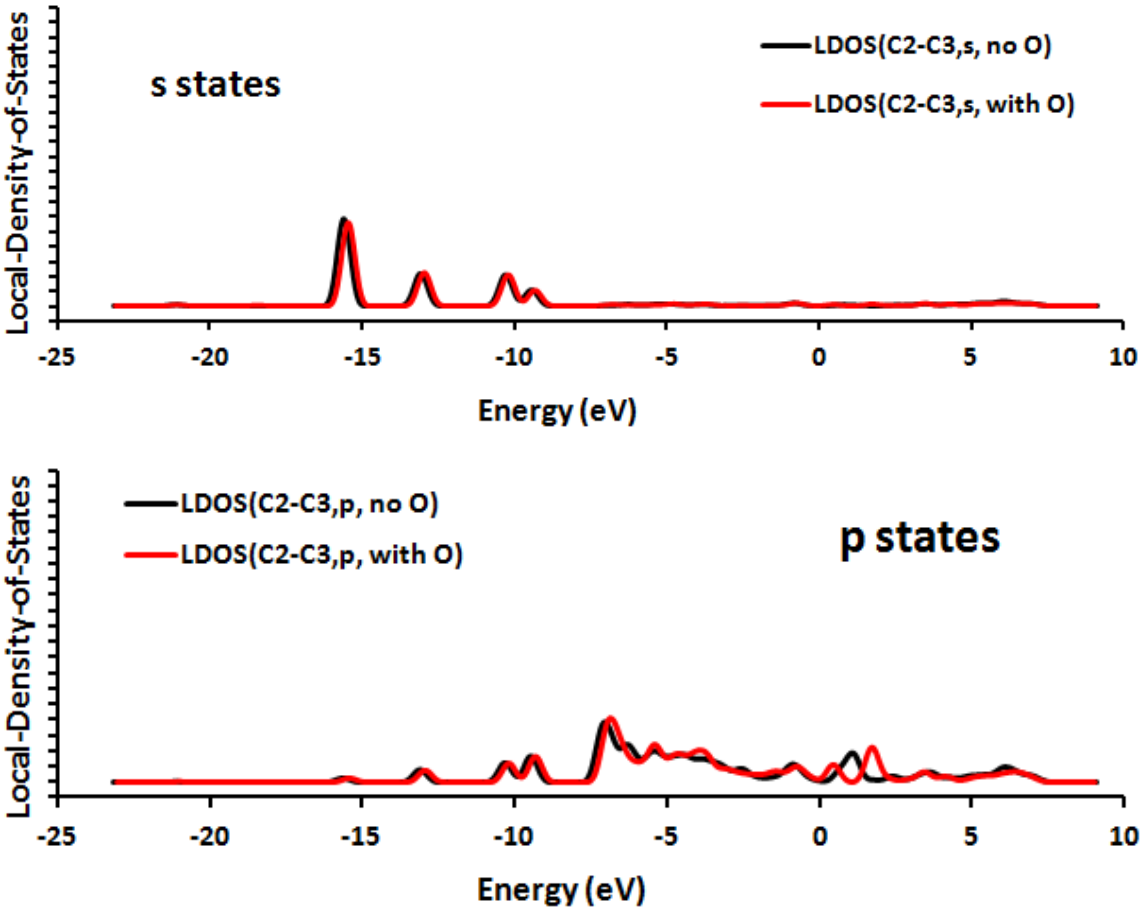

Figure S2b. LDOS plots for **E-(s)-trans-di-σ-crotonaldehyde** on $Au_{13}O_6$ (with and without neighbouring hollow O adatom) projected onto bonding allylic carbon atoms.

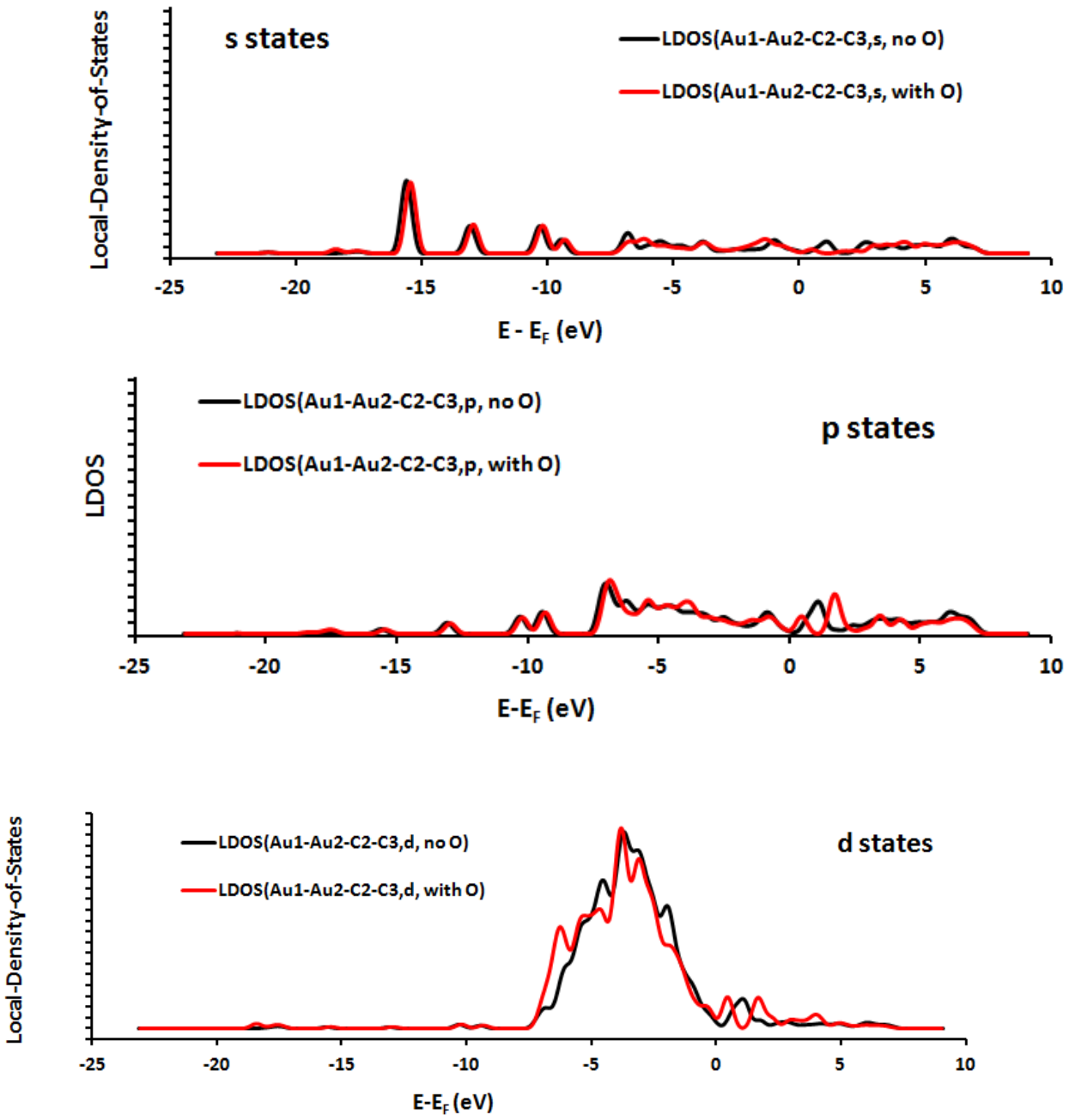

Figure S2c. LDOS plots for **E-(s)-trans-di-σ-crotonaldehyde** on $Au_{13}O_6$ (with and without neighbouring hollow O adatom) projected onto gold/allylic carbon bonding unit.

LDOS difference plots

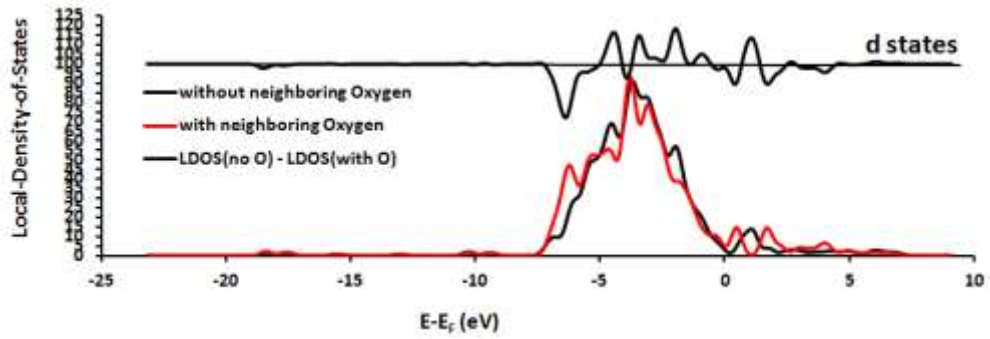

Figure S2d. Difference between LDOS plots for **E-(s)-trans-di-σ-crotonaldehyde** on $Au_{13}O_6$ adsorbed with or without neighbouring hollow O adatom.