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Rhenium(V) complexes containing mono- and tridentate imido ligands: crystal structures, spectroscopic results and DFT optimization

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Table S1. Selected experimental and optimized (PBE1PBE) bond lengths (Å) and angles (°) for the complexes **1** and **2**.

1

	Exp.	**PBE1PBE**		**Exp.**	**PBE1PBE**
Re(1) – Br(1)	2.508(1)	2.577	Re(2) – Br(2)	2.500(1)	2.553
Re(1) – O(1)	1.924(6)	1.949	Re(2) – O(2)	1.896(6)	1.962
Re(1) – N(11)	2.174(8)	2.173	Re(2) – N(21)	2.191(9)	2.185
Re(1) – N(12)	1.772(7)	1.757	Re(2) – N(22)	1.773(6)	1.751
Re(1) – P(11)	2.486(2)	2.509	Re(2) – P(21)	2.483(3)	2.506
Re(1) – P(12)	2.491(2)	2.506	Re(2) – P(22)	2.488(2)	2.519
N(11) – C(1)	1.28(1)	1.308	N(21) – C(2)	1.24(1)	1.304
O(1)-Re(1)-N(12)	159.2(3)	158.92	O(2)-Re(2)-N(22)	158.3(3)	158.27
P(11)-Re(1)-P(12)	176.77(7)	174.23	P(21)-Re(2)-P(22)	179.09(7)	171.94
O(1)-Re(1)-N(11)	83.5(3)	82.92	O(2)-Re(2)-N(21)	84.1(3)	82.41
N(11)-Re(1)-N(12)	75.7(3)	76.02	N(21)-Re(2)-N(22)	74.2(3)	75.87
Br(1)-Re(1)-N(11)	176.4(2)	178.08	Br(2)-Re(2)-N(21)	178.7(2)	178.02
Br(1)-Re(1)-O(1)	92.9(2)	95.87	Br(2)-Re(2)-O(2)	97.3(2)	99.31

2

Re(1)–N(12)	1.725(3)	1.757	Re(2)- N(22)	1.721(4)	1.758
Re(1)–O(11)	2.013(3)	2.048	Re(2)–O(21)	2.001(3)	2.051
Re(1)–N(11)	2.196(5)	2.188	Re(2)–N(21)	2.219(4)	2.187
Re(1)–I(1)	2.723(4)	2.777	Re(2)–I(2)	2.718(4)	2.775

Re(1)–P(11)	2.499(1)	2.474	Re(2)–P(21)	2.479(1)	2.471
Re(1)–P(12)	2.492(1)	2.476	Re(2)–P(22)	2.494(1)	2.474
O(11)-Re(1)-N(11)	76.8(2)	75.70	O(21)-Re(2)-N(21)	76.0(1)	75.81
P(11)-Re(1)-P(12)	176.03(4)	177.26	P(21)-Re(2)-P(22)	173.23(4)	177.44
N(12)-Re(1)-O(11)	169.2(2)	165.83	N(22)-Re(2)-O(21)	168.9(2)	165.84
I(1)-Re(1)-N(11)	166.5(1)	163.74	I(2)-Re(2)-N(21)	165.4(1)	163.62
I(1)-Re(1)-O(11)	89.8(1)	88.18	I(2)-Re(2)-O(21)	89.5(1)	87.89

Table S2. Energy(eV) and wavelength (nm) of experimental absorption bands and the most important electronic transitions calculated with PBE1PBE for complexes **1** and **2**.

		1			
Excitations	**Character**	**λ(nm)**	**E(eV)**	***f***	**Exp. λ(nm) ; ε (mm^{-1})**
H-7 ⟶L	$\pi(PPh_3) \longrightarrow d_{xy}$, π(L), π^*(L)	363.76	3.4084	0.1574	407; 5.662
H-6⟶ L	d_{xz}, π(L), $\pi(PPh_3)$, π(N), π(Br) ⟶ d_{xy}, π(L), π^*(L)				
H-1⟶ L+3	d_{xz}, π(L), π(Br), π(O) ⟶ d_{xz} $\pi(PPh_3)$, $\pi^*(PPh_3)$	284.03	4.3652	0.2165	293
H-16⟶ L+1	π(Br), $\pi(PPh_3)$, $\pi^*(PPh_3)$⟶ d_{yz}, π(N), π(Br), π(O)	276.06	4.4912	0.1155	293
H-15⟶ L+1	π(Br), $\pi(PPh_3)$, $\pi^*(PPh_3)$, π(N) ⟶ d_{yz}, π(N), π(Br), π(O)				
		2			
Excitations	**Character**	**λ(nm)**	**E(eV)**	***f***	**Exp. λ(nm) ; ε (mm^{-1})**
H-1⟶ L	π(L), π(N), π(O) ⟶ d_{xy}, π(L), π(N) , π(O)	413.56	2.9980	0.1579	433; 4.269
H-3⟶L+2	π(I), π(L), $\pi(PPh_3)$, $\pi^*(PPh_3)$⟶ d_{xz}, $\pi(PPh_3)$, $\pi^*(PPh_3)$	265.94	4.6621	0.0936	301

H-highest occupied molecular orbital; L-lowest unoccupied molecular orbital; *f*-oscillator strength; ε-molar extinction coefficient.

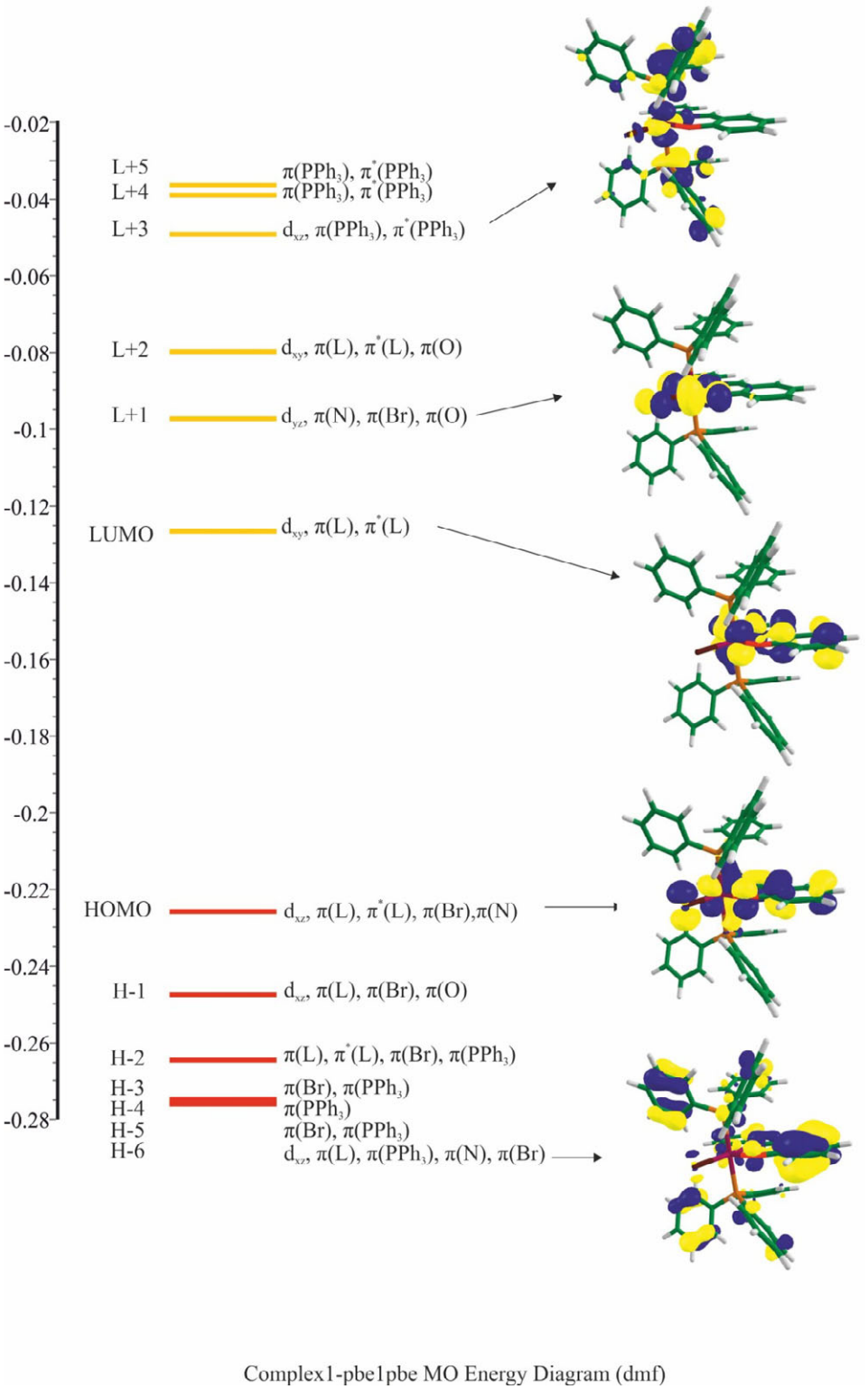

Figure S1. The energy (a.u.), character and some contours of the molecular orbitals of **1** calculated with the PBE1PBE functional (Basis set: LANL2DZ for Re, 6-31G for Br, C, O, N, H and 6-31+G(d) for P). Positive orbital contour are represented in blue and negative ones in yellow.

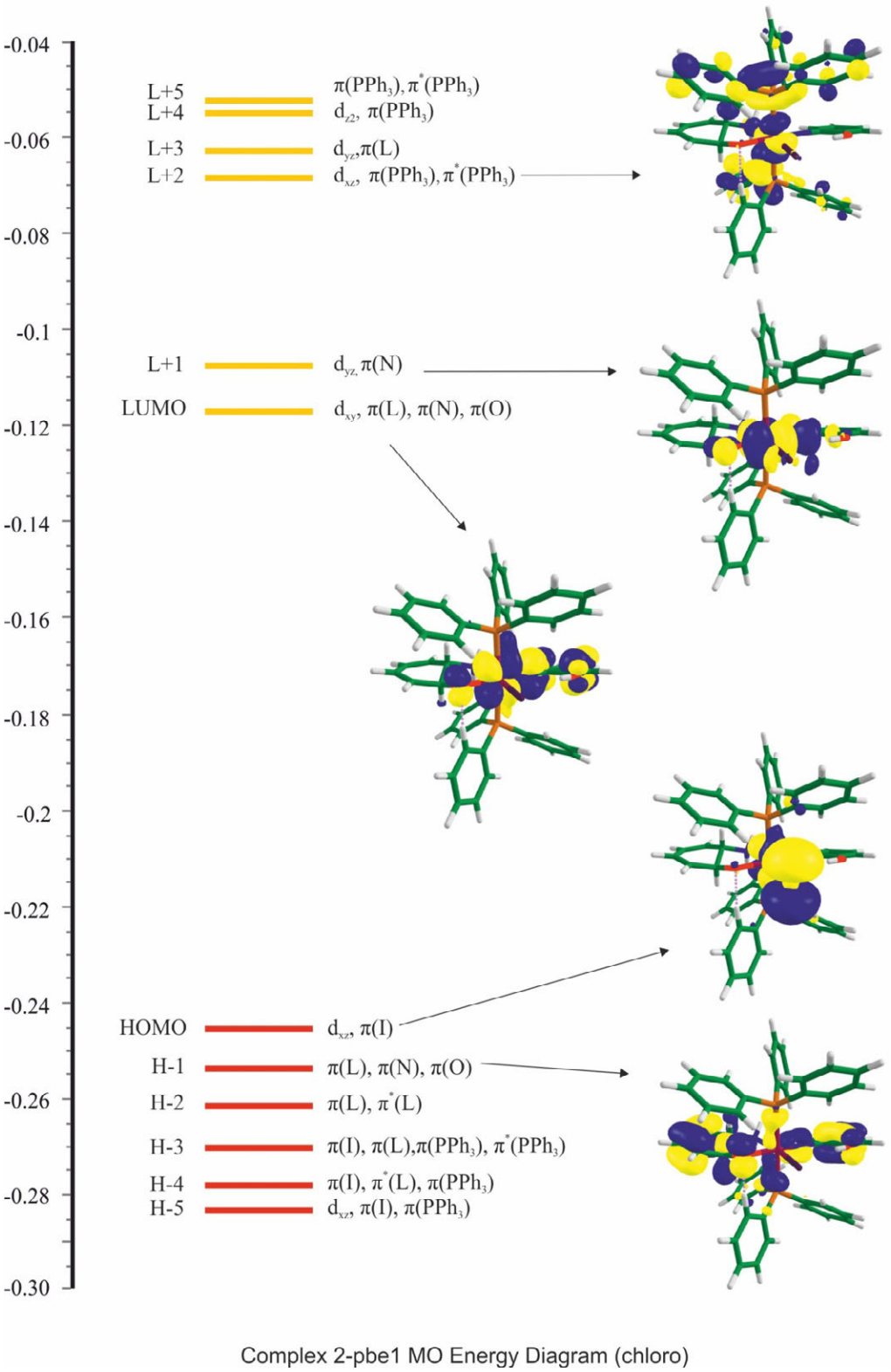

Figure S2. The energy (a.u.), character and some contours of the molecular orbitals of **2** calculated with the PBE1PBE functional. Positive orbital contour are represented in blue and negative ones in yellow.

5. Input File for Complex 1 and Optimized Cartesian Coordinates (Å) of Structures

The gas phase geometries of complexes **1** and **2** were optimized with the DFT method using both the B3LYP and PBE1PBE functionals of Gaussian 09. For both the B3LYP and PBE1PBE functionals, the calculations were performed by using the ECP basis set (LANL2DZ) for the rhenium atom, 6-31G for bromine, carbon, oxygen, nitrogen and hydrogen atoms and 6-31+G(d) for the phosphorus atoms. An additional d function with exponent α=0.3811 and an f function with exponent α=2.0330 on the rhenium atom is added. The positive vibrational frequencies of the optimized structures have confirmed the optimized structures as being true minima. The electronic transition energies have been obtained with the time-dependent density functional theory (TD-DFT) in a polar medium described by the dielectric constant ε=36.7 (DMF). The PCM methodology was used to take into account the effect of the medium. Chemcraft was used to reproduce the molecular orbitals (http://www.chemcraftprog.com/).

Input File for Complex 1- (B3LYP)

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#B3lyp/gen pseudo=read Test Opt  scf=(MaxCycle=200,qc,direct)
0 1
 Re   5.402  -5.831  -0.494
 Br   6.896  -3.806  -0.514
  O   4.975  -5.922  -2.435
  N   4.064  -7.699  -0.506
  C   3.390  -8.249  -1.498
  H   2.772  -9.149  -1.337
  C   4.134  -6.594  -3.252
  C   2.514  -7.900  -5.102
  C   4.061  -6.121  -4.579
  C   3.392  -7.722  -2.845
  C   2.580  -8.365  -3.805
  C   3.252  -6.775  -5.489
  H   4.640  -5.237  -4.875
  H   1.988  -9.242  -3.515
  H   3.185  -6.410  -6.521
  H   1.876  -8.407  -5.835
  P   7.451  -7.056  -1.203
  P   3.475  -4.276  -0.259
  C   8.568  -6.328  -2.486
  C  10.255  -5.208  -4.403
  C   9.829  -6.871  -2.713
  C   8.156  -5.217  -3.216
  C   8.997  -4.659  -4.175
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H 8.670 -3.780 -4.740
H 11.664 -6.745 -3.840
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C 10.494 -7.700 2.248
C 9.401 -8.544 0.273
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C 6.970 -10.243 -3.807
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H 6.430 -12.289 -3.377
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C 1.269 -5.889 0.490
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C -0.086 -5.576 -1.915
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C 2.303 -1.894 -1.209
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H 1.527 -2.053 -0.442
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C	3.231	-2.361	3.954
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C	4.515	-3.251	2.120
C	4.463	-2.663	3.377
C	2.056	-2.643	3.268
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H	5.492	-3.471	1.665
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N	5.373	-6.413	1.150
Re	-2.178	-2.178	1.612
O	-1.456	-2.613	3.167
O	-0.916	-2.271	0.371
O	-2.807	-0.521	1.686
O	-3.466	-3.318	1.218
Re	-4.342	6.353	1.069
Br	-1.944	7.142	0.880
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H	-7.090	6.266	-5.212
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C	-0.388	2.641	-2.354

C -2.037 2.118 -0.677
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H -0.105 4.741 -2.769
H -0.894 0.630 -1.739
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C -2.418 2.159 2.774
C -2.263 4.521 3.204
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Br  -9.930   6.335  -1.053
 H  -8.257   5.890  -0.742

Re 0
LANL2DZ
****
Br C O N H 0
6-31G
****
P 0
6-31+G(d)
****

Re 0
LANL2DZ

Re 0
D    1 1.00
0.38110000000D+00  0.1000000000D+01
F    1 1.00
2.0330000000D+00  0.1000000000D+01
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Optimized Cartesian Coordinates (Å)

Complex 1-Monomer (B3LYP; HF=-5408.1087091 a.u.)

Re	-0.000051	-0.171107	-0.286038
Br	-0.000381	0.048145	-2.849581
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C	0.000081	4.340308	3.394347
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C	0.000066	2.057994	2.519019
C	0.000102	2.965582	3.605629
C	0.000017	4.832735	2.078395
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H	0.000169	2.570970	4.617973
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C	-3.938589	-1.880741	1.283995
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C	4.405831	2.104965	-0.047182
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H	4.922580	1.480458	0.671991
H	5.830166	3.708067	0.141801
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H	4.685919	5.168028	-1.517870
C	3.302750	-1.094757	-1.678656
C	4.484698	-2.753719	-3.620842
C	2.689692	-2.306925	-2.050901
C	4.510911	-0.719654	-2.298863
C	5.095570	-1.546414	-3.263859
C	3.282620	-3.131598	-3.012304
H	1.743182	-2.595079	-1.609478
H	4.992188	0.215981	-2.038637
H	6.023253	-1.243585	-3.737800
H	2.797777	-4.059949	-3.295657
H	4.937774	-3.390712	-4.373139
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C	4.436751	-1.509998	3.630865
C	3.299514	0.204815	2.344364
C	3.938416	-1.880347	1.283762
C	4.479075	-2.326353	2.496466
C	3.846971	-0.241520	3.550583
H	2.860087	1.195815	2.296162
H	3.993177	-2.519679	0.410364
H	4.941836	-3.306346	2.547123
H	3.825480	0.404400	4.422771
H	4.866441	-1.852882	4.566203
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C	0.001351	-2.216861	3.644267
C	0.000404	-2.592361	1.245744
C	0.000570	-3.976895	1.420569
C	0.001512	-3.610966	3.822620
H	0.001796	-1.572937	4.515852
H	0.000308	-4.631396	0.557193
H	0.001985	-4.013171	4.829426

H	0.001231	-5.555034	2.889553
N	0.000082	-1.909848	0.032433

Complex 1-Monomer (PBE1PBE; HF=-5405.0542997 a.u.**)**

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C	-0.000487	2.534721	1.205438
C	-0.001135	4.234476	3.444063
C	-0.000644	3.920748	1.031828
C	-0.000599	1.984829	2.510257
C	-0.000953	2.858389	3.618395
C	-0.000970	4.759406	2.144387
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H	-0.001102	5.834051	1.998169
H	-0.001397	4.895879	4.301838
P	-2.500500	-0.021510	-0.376927
P	2.500345	-0.020728	-0.377292
C	-3.273210	-1.041590	-1.677699
C	-4.510212	-2.652044	-3.608972
C	-4.524261	-0.681960	-2.205234
C	-2.642881	-2.209396	-2.135484
C	-3.264211	-3.011345	-3.093048
C	-5.137296	-1.486171	-3.165771
H	-5.014620	0.227717	-1.875669
H	-1.661038	-2.476524	-1.760688
H	-2.767095	-3.908143	-3.446991
H	-6.101078	-1.197790	-3.571210
H	-4.986868	-3.272667	-4.360151
C	-3.236554	-0.630420	1.182724
C	-4.227892	-1.606431	3.624431
C	-3.195784	0.166782	2.341272
C	-3.778570	-1.922393	1.266349
C	-4.268466	-2.405508	2.482035
C	-3.692695	-0.317419	3.550452
H	-2.795546	1.175266	2.293187
H	-3.831239	-2.546946	0.380950
H	-4.692387	-3.402819	2.529647
H	-3.676294	0.316266	4.431527
H	-4.620380	-1.979571	4.564384
C	-3.171295	1.656789	-0.617624
C	-4.229236	4.202938	-1.134985
C	-2.544356	2.511911	-1.540188

C	-4.339348	2.087882	0.034607
C	-4.861006	3.356548	-0.222919
C	-3.074980	3.776228	-1.794807
H	-1.656423	2.181135	-2.066693
H	-4.845178	1.436519	0.739079
H	-5.764362	3.677826	0.284534
H	-2.588933	4.424784	-2.515962
H	-4.639025	5.186956	-1.336688
C	3.170576	1.657798	-0.618025
C	4.227581	4.204279	-1.135631
C	2.543209	2.512677	-1.540541
C	4.338576	2.089298	0.034010
C	4.859771	3.358139	-0.223635
C	3.073371	3.777158	-1.795279
H	1.655315	2.181570	-2.066903
H	4.844714	1.438126	0.738442
H	5.763095	3.679732	0.283674
H	2.587020	4.425536	-2.516390
H	4.637013	5.188425	-1.337434
C	3.273241	-1.040595	-1.678103
C	4.510678	-2.650824	-3.609280
C	2.643065	-2.208412	-2.136071
C	4.524353	-0.680837	-2.205408
C	5.137603	-1.484934	-3.165904
C	3.264610	-3.010245	-3.093592
H	1.661164	-2.475617	-1.761478
H	5.014591	0.228852	-1.875694
H	6.101427	-1.196446	-3.571169
H	2.767620	-3.907055	-3.447680
H	4.987503	-3.271373	-4.360412
C	3.236819	-0.629404	1.182234
C	4.228823	-1.604970	3.623834
C	3.195728	0.167769	2.340811
C	3.779491	-1.921087	1.265781
C	4.269728	-2.403992	2.481419
C	3.692951	-0.316221	3.549936
H	2.794974	1.176048	2.292759
H	3.832397	-2.545582	0.380351
H	4.694164	-3.401087	2.528964
H	3.676291	0.317415	4.431041
H	4.621569	-1.977930	4.563751
C	0.000991	-1.754210	2.246307
C	0.002133	-4.531737	2.563390
C	0.002030	-2.290417	3.527023
C	0.000749	-2.616162	1.129492
C	0.001267	-3.999823	1.271387
C	0.002554	-3.684126	3.673672
H	0.002616	-1.666392	4.413031

H	0.001054	-4.634596	0.393463
H	0.003353	-4.108013	4.671455
H	0.002554	-5.606143	2.704430
N	0.000282	-1.902824	-0.058165

Complex 1-Dimer (B3LYP; HF= -13768.0069094 a.u.**)**

Re	-7.854886	0.256128	-0.304407
Br	-8.460810	0.589103	-2.794286
O	-7.078693	2.031107	0.062893
N	-7.394772	-0.055076	1.842598
C	-6.877559	0.799027	2.687440
H	-6.731293	0.482868	3.718579
C	-6.524119	2.714115	1.098455
C	-5.398314	4.193887	3.214898
C	-6.024086	4.001847	0.868367
C	-6.445915	2.142962	2.396147
C	-5.881106	2.907989	3.441218
C	-5.467353	4.734080	1.921262
H	-6.067814	4.403262	-0.136383
H	-5.818361	2.470746	4.433501
H	-5.081172	5.729588	1.729622
H	-4.964371	4.766282	4.026101
P	-10.130029	1.344102	0.257757
P	-5.500196	-0.534951	-0.922065
C	-10.594461	2.806746	-0.757684
C	-11.292276	5.080190	-2.262585
C	-11.944140	3.082561	-1.050345
C	-9.597402	3.678837	-1.236055
C	-9.948785	4.810439	-1.979368
C	-12.288085	4.213324	-1.798665
H	-12.725209	2.414030	-0.706666
H	-8.553841	3.461512	-1.045045
H	-9.171476	5.471270	-2.349049
H	-13.331302	4.411021	-2.022622
H	-11.560855	5.953965	-2.847369
C	-11.534253	0.169787	0.061231
C	-13.690370	-1.592740	-0.366430
C	-12.642513	0.169322	0.931880
C	-11.525250	-0.719583	-1.032659
C	-12.598819	-1.590873	-1.242826
C	-13.710391	-0.710283	0.719072
H	-12.676050	0.848786	1.775707
H	-10.691091	-0.717866	-1.723993
H	-12.579878	-2.265660	-2.092297
H	-14.555964	-0.700622	1.399341
H	-14.519932	-2.272861	-0.530445
C	-10.254357	1.942816	1.996905
C	-10.316202	2.808870	4.681422

C	-10.235063	3.315422	2.308257
C	-10.299679	1.009242	3.054431
C	-10.337491	1.439740	4.383707
C	-10.262586	3.742521	3.641866
H	-10.202507	4.051591	1.513628
H	-10.321276	-0.054217	2.839743
H	-10.389225	0.708542	5.184403
H	-10.249440	4.804678	3.863447
H	-10.346838	3.142525	5.713550
C	-4.560168	-0.948719	0.602143
C	-3.165913	-1.544339	2.976474
C	-4.529191	-2.263002	1.104840
C	-3.892963	0.067117	1.314723
C	-3.205815	-0.229830	2.495131
C	-3.827365	-2.559523	2.278726
H	-5.007472	-3.067476	0.558236
H	-3.876357	1.081699	0.932160
H	-2.674115	0.558813	3.018576
H	-3.752609	-3.587371	2.613044
H	-2.595809	-1.782188	3.868365
C	-4.434433	0.693740	-1.783226
C	-2.780865	2.479270	-3.193911
C	-4.994291	1.771803	-2.494473
C	-3.032770	0.516793	-1.783454
C	-2.217698	1.408120	-2.489918
C	-4.168142	2.658744	-3.193938
H	-6.066435	1.908732	-2.520568
H	-2.563368	-0.302701	-1.245650
H	-1.143523	1.255922	-2.486170
H	-4.612908	3.481187	-3.745726
H	-2.142328	3.164288	-3.743090
C	-5.468696	-2.073167	-1.930242
C	-5.343168	-4.417071	-3.480768
C	-4.245400	-2.757642	-2.097027
C	-6.626098	-2.574995	-2.554791
C	-6.557590	-3.739552	-3.328544
C	-4.186072	-3.927017	-2.862705
H	-3.338818	-2.401909	-1.621439
H	-7.568923	-2.055404	-2.457455
H	-7.455420	-4.111223	-3.812881
H	-3.236143	-4.444734	-2.943946
H	-5.296675	-5.323387	-4.076502
C	-7.758790	-1.385812	2.258404
C	-8.607835	-4.030533	2.639903
C	-7.603601	-1.977459	3.509889
C	-8.338801	-2.128143	1.200353
C	-8.764066	-3.445220	1.376551
C	-8.033646	-3.302838	3.690439

H	-7.142629	-1.452359	4.338235
H	-9.193904	-3.988695	0.544279
H	-7.906346	-3.770191	4.660507
H	-8.924348	-5.054304	2.802002
N	-8.396804	-1.386922	0.024235
Re	-0.680708	-3.552441	-0.293336
O	-1.193249	-4.529448	-1.659009
O	-1.389870	-1.941098	-0.459007
O	1.073240	-3.421963	-0.262697
O	-1.260813	-4.280728	1.192142
Re	7.175931	0.476029	-0.721175
Br	6.475264	1.832712	-2.839351
O	6.367410	1.699184	0.577073
N	7.788281	-0.602375	1.101125
C	7.572973	-0.273817	2.353287
C	6.271498	1.846102	1.929104
C	6.085455	2.216360	4.709471
C	5.570316	2.942993	2.441521
C	6.871226	0.907517	2.806802
C	6.778153	1.116940	4.202189
C	5.478784	3.121411	3.826783
H	5.113809	3.637998	1.748087
H	7.286926	0.412778	4.859083
H	4.936119	3.977713	4.215488
H	6.023738	2.369603	5.780913
P	4.914295	-0.728464	-0.731584
P	9.318074	1.881938	-0.631711
C	3.414752	0.335064	-0.566633
C	1.092295	1.917396	-0.387371
C	2.166723	-0.254657	-0.273206
C	3.482487	1.726567	-0.766987
C	2.326019	2.509897	-0.675267
C	1.012756	0.533012	-0.188837
H	2.073743	-1.322096	-0.109244
H	4.426809	2.194796	-1.002977
H	2.394781	3.581747	-0.835718
H	0.063164	0.050437	0.018426
H	0.195963	2.527727	-0.321707
C	4.620576	-1.796936	-2.206395
C	4.114649	-3.383028	-4.478179
C	3.593989	-2.766192	-2.187836
C	5.388292	-1.635840	-3.375162
C	5.133870	-2.425929	-4.502631
C	3.346797	-3.550000	-3.319469
H	2.977950	-2.929227	-1.310442
H	6.167605	-0.887401	-3.414368
H	5.731208	-2.285180	-5.398218
H	2.549293	-4.285051	-3.286088

H	3.917496	-3.992844	-5.354730
C	4.801841	-1.886499	0.691619
C	4.837760	-3.595042	2.931933
C	4.308982	-1.447217	1.935441
C	5.319695	-3.192139	0.588827
C	5.332111	-4.039758	1.701168
C	4.326957	-2.297162	3.045594
H	3.907823	-0.445251	2.038172
H	5.701909	-3.553030	-0.359582
H	5.727736	-5.045396	1.604022
H	3.943974	-1.944390	3.997473
H	4.853406	-4.251523	3.795392
C	10.680949	1.132454	0.351852
C	12.647887	-0.194631	1.873609
C	10.532053	0.972419	1.745940
C	11.841581	0.625064	-0.265898
C	12.819504	-0.026655	0.495615
C	11.500042	0.304954	2.502259
H	9.653756	1.356037	2.252332
H	11.982983	0.732038	-1.334781
H	13.708778	-0.410529	0.004932
H	11.316277	0.128036	3.558025
H	13.395688	-0.722444	2.456637
C	9.070758	3.571531	0.053495
C	8.649785	6.189601	1.001488
C	7.970938	4.328141	-0.401725
C	9.955886	4.144855	0.985776
C	9.742490	5.445770	1.457687
C	7.768319	5.628683	0.068892
H	7.284358	3.902329	-1.124518
H	10.806719	3.580284	1.347873
H	10.431516	5.872487	2.179620
H	6.920160	6.201488	-0.292805
H	8.485946	7.197999	1.368656
C	10.074835	2.168243	-2.286773
C	11.303545	2.540425	-4.792130
C	9.999238	1.168246	-3.274707
C	10.768027	3.359416	-2.572332
C	11.376781	3.543055	-3.818769
C	10.615445	1.353362	-4.516452
H	9.446047	0.257527	-3.077728
H	10.829421	4.144168	-1.826728
H	11.904525	4.468419	-4.027095
H	10.545339	0.576183	-5.270770
H	11.773833	2.685399	-5.759671
C	8.534428	-1.790828	0.777279
C	9.905927	-3.990864	-0.281287
C	9.130873	-2.695698	1.654026

C	8.651089	-1.974730	-0.623067
C	9.325559	-3.071949	-1.164150
C	9.815172	-3.793660	1.104166
H	9.115054	-2.551717	2.734807
H	9.391076	-3.190028	-2.239401
H	10.287419	-4.498926	1.779525
H	10.436074	-4.852430	-0.672313
N	8.040941	-0.942100	-1.326945
Br	9.371160	-1.408189	5.103970
H	7.989206	-0.895295	3.156290

Complex 1-Dimer (PBE1PBE; HF=-13761.2188727 a.u.**)**

Re	-7.455499	0.165764	-0.226513
Br	-8.561259	-0.474337	-2.437090
O	-6.570664	1.825318	-0.783520
N	-6.567535	0.680892	1.701831
C	-5.887444	1.748703	2.015642
H	-5.538145	1.854488	3.040953
C	-5.830495	2.816116	-0.244572
C	-4.318825	4.920418	0.840512
C	-5.369186	3.844688	-1.069239
C	-5.515749	2.819992	1.134244
C	-4.760990	3.887555	1.656557
C	-4.621041	4.888217	-0.526181
H	-5.593113	3.799427	-2.127828
H	-4.517246	3.886925	2.715111
H	-4.265514	5.680195	-1.176612
H	-3.735454	5.734021	1.254312
P	-9.465091	1.611931	0.237416
P	-5.341067	-1.005438	-0.886809
C	-10.117266	2.556480	-1.183010
C	-11.098738	4.064935	-3.330950
C	-11.485088	2.859825	-1.269596
C	-9.246252	3.006411	-2.188218
C	-9.738565	3.761563	-3.252850
C	-11.970740	3.611127	-2.339901
H	-12.172403	2.500262	-0.511154
H	-8.194223	2.747386	-2.144266
H	-9.060502	4.098876	-4.029658
H	-13.030536	3.834659	-2.401673
H	-11.479462	4.644416	-4.165461
C	-10.887172	0.641405	0.850622
C	-13.110566	-0.864266	1.662503
C	-11.756994	1.133898	1.837677
C	-11.148580	-0.610057	0.267391
C	-12.256555	-1.354046	0.672284
C	-12.860126	0.380083	2.242399
H	-11.574495	2.101743	2.292219

H	-10.494813	-0.989309	-0.510409
H	-12.451292	-2.316346	0.210910
H	-13.523513	0.768934	3.007901
H	-13.969278	-1.447755	1.977794
C	-9.172103	2.880119	1.524023
C	-8.581059	4.777330	3.510677
C	-9.053603	4.239441	1.197904
C	-8.988355	2.482294	2.861072
C	-8.701289	3.425750	3.846578
C	-8.756783	5.179990	2.187010
H	-9.196484	4.564811	0.173129
H	-9.083014	1.435168	3.133885
H	-8.578161	3.106868	4.876755
H	-8.669973	6.227850	1.920028
H	-8.358940	5.510919	4.278574
C	-4.114466	-0.850118	0.455862
C	-2.271037	-0.537392	2.546566
C	-3.966342	-1.849743	1.428142
C	-3.334653	0.314816	0.548430
C	-2.422489	0.470582	1.590386
C	-3.041784	-1.696568	2.463195
H	-4.532048	-2.772100	1.352801
H	-3.413905	1.084541	-0.212588
H	-1.803489	1.361268	1.633424
H	-2.881171	-2.510127	3.160045
H	-1.529522	-0.435811	3.332006
C	-4.471792	-0.325894	-2.343807
C	-3.107293	0.635075	-4.595698
C	-5.155170	0.409096	-3.324800
C	-3.096007	-0.581847	-2.500735
C	-2.423841	-0.099533	-3.624679
C	-4.471888	0.885307	-4.444785
H	-6.217446	0.592460	-3.226300
H	-2.539630	-1.155061	-1.761238
H	-1.363919	-0.304788	-3.732816
H	-5.011770	1.444167	-5.202643
H	-2.578948	1.004620	-5.468828
C	-5.534211	-2.801671	-1.147171
C	-5.750782	-5.565345	-1.551123
C	-4.379241	-3.594203	-1.281026
C	-6.797828	-3.406473	-1.222419
C	-6.900180	-4.783580	-1.427895
C	-4.488726	-4.971367	-1.475163
H	-3.390714	-3.151125	-1.210478
H	-7.694656	-2.806572	-1.138396
H	-7.881890	-5.241772	-1.494739
H	-3.579229	-5.559779	-1.543402
H	-5.836038	-6.636465	-1.704031

C	-6.829434	-0.330824	2.682341
C	-7.578668	-2.511386	4.262321
C	-6.391819	-0.396063	3.999063
C	-7.636900	-1.365699	2.163623
C	-8.017693	-2.457052	2.937267
C	-6.775064	-1.493026	4.781704
H	-5.742002	0.358755	4.426269
H	-8.628346	-3.238940	2.503224
H	-6.427048	-1.555065	5.806591
H	-7.852601	-3.353662	4.886586
N	-7.943398	-1.141225	0.831646
Re	-0.643015	-3.913979	0.053979
O	-1.257667	-5.288746	-0.826826
O	-1.367196	-2.456132	-0.610395
O	1.095819	-3.817352	-0.097587
O	-1.095038	-4.055045	1.731156
Re	6.821361	0.369606	-0.798417
Br	6.412307	1.235625	-3.190566
O	5.793984	1.762744	0.096099
N	7.187634	-0.293158	1.238096
C	6.779803	0.248407	2.356473
C	5.503989	2.165711	1.354869
C	4.908881	3.046632	3.949579
C	4.716597	3.302934	1.539384
C	5.986928	1.447262	2.470944
C	5.688340	1.908244	3.768692
C	4.422455	3.735245	2.833451
H	4.353863	3.829873	0.665751
H	6.111375	1.362867	4.613243
H	3.813681	4.623981	2.968192
H	4.688677	3.398272	4.950888
P	4.673561	-0.926982	-0.833192
P	8.831634	1.860227	-0.677618
C	3.134768	0.032392	-1.084351
C	0.744442	1.419507	-1.557082
C	1.895082	-0.566150	-0.796093
C	3.164279	1.334132	-1.606005
C	1.971351	2.021231	-1.839866
C	0.706039	0.125045	-1.033081
H	1.842608	-1.570692	-0.388668
H	4.112143	1.799807	-1.840823
H	2.006920	3.025124	-2.251818
H	-0.235334	-0.367759	-0.811862
H	-0.182165	1.952495	-1.751059
C	4.622300	-2.291681	-2.050717
C	4.478735	-4.346903	-3.952509
C	3.665265	-3.314680	-1.918289
C	5.505032	-2.310303	-3.141266

C	5.430228	-3.335381	-4.086387
C	3.598465	-4.333435	-2.868531
H	2.967977	-3.343677	-1.085779
H	6.233758	-1.518039	-3.259962
H	6.114616	-3.335993	-4.928782
H	2.851478	-5.111574	-2.751809
H	4.421596	-5.141693	-4.689820
C	4.423778	-1.755930	0.773477
C	4.272074	-2.919159	3.323129
C	3.753420	-1.098239	1.816899
C	5.017028	-3.003497	1.023201
C	4.935543	-3.581386	2.289935
C	3.680253	-1.677939	3.082958
H	3.287695	-0.134129	1.641300
H	5.533491	-3.528877	0.226718
H	5.394517	-4.547811	2.468530
H	3.165759	-1.156818	3.883127
H	4.220086	-3.364181	4.310647
C	10.026768	1.353054	0.607034
C	11.729549	0.361762	2.606716
C	9.685030	1.472666	1.966816
C	11.242896	0.739280	0.264469
C	12.090242	0.255110	1.263345
C	10.523263	0.971467	2.961885
H	8.753013	1.945690	2.259599
H	11.527233	0.636662	-0.777041
H	13.028017	-0.215456	0.985274
H	10.194491	1.002666	3.997208
H	12.377065	-0.039619	3.379221
C	8.444385	3.614835	-0.352512
C	7.824570	6.322772	0.030313
C	7.413766	4.218379	-1.094364
C	9.162624	4.382510	0.576772
C	8.849542	5.729928	0.767390
C	7.111809	5.565810	-0.902697
H	6.859327	3.633885	-1.821311
H	9.961681	3.930278	1.153624
H	9.408920	6.311930	1.492460
H	6.317379	6.023399	-1.483422
H	7.582577	7.370100	0.180508
C	9.820779	1.891897	-2.215611
C	11.409712	1.887206	-4.525333
C	9.901155	0.743641	-3.018304
C	10.538628	3.039481	-2.585029
C	11.327741	3.035330	-3.735813
C	10.697188	0.742658	-4.163756
H	9.327465	-0.137944	-2.753521
H	10.476203	3.936425	-1.977769

H	11.875104	3.929758	-4.014991
H	10.748194	-0.148543	-4.780544
H	12.021262	1.886529	-5.421896
C	8.017308	-1.460239	1.271362
C	9.613027	-3.716858	0.883878
C	8.505691	-2.131726	2.386129
C	8.351721	-1.902649	-0.026914
C	9.140019	-3.031346	-0.236679
C	9.305400	-3.262406	2.170588
H	8.315186	-1.784525	3.404035
H	9.371100	-3.350635	-1.246016
H	9.695847	-3.789924	3.034019
H	10.229312	-4.599609	0.754804
N	7.812071	-1.068980	-0.991599
Br	8.101203	-0.259083	5.501921
H	7.093585	-0.185010	3.317512

Complex 2-Monomer (B3LYP; HF=-9766.2078641 a.u.**)**

Re	0.004804	-0.075224	0.024729
I	0.051943	0.592558	-2.698116
O	0.044595	-2.002029	-0.453319
N	-0.090635	1.543461	0.703265
C	-0.238573	2.774225	1.286077
C	-0.517247	5.331739	2.406209
C	-0.488766	2.928721	2.673021
C	-0.136396	3.933247	0.464913
C	-0.274811	5.202249	1.041326
C	-0.627501	4.193500	3.228798
H	-0.574413	2.039797	3.289486
H	-0.191685	6.066324	0.393688
H	-0.820981	4.304178	4.289425
H	-0.623990	6.320639	2.837938
O	0.097882	3.877282	-0.882766
H	0.182989	2.969061	-1.255461
N	0.034190	-1.150633	2.031192
H	0.661353	-0.656994	2.666768
H	-0.911578	-1.147536	2.427029
C	0.512535	-2.555650	1.808372
C	0.343098	-4.868732	2.583191
C	0.325316	-4.412639	0.171181
C	0.520051	-5.287891	1.180848
C	-0.167210	-3.031529	0.527960
C	0.297546	-3.560598	2.920308
H	0.278795	-5.637207	3.347083
H	0.417439	-4.679415	-0.875074
H	0.793864	-6.318722	0.982435
H	-1.255953	-3.103203	0.718113
H	0.226374	-3.229370	3.952095

H	1.588835	-2.475414	1.598262
P	2.588816	-0.067216	-0.027835
P	-2.571003	-0.212939	-0.073193
C	-3.248047	-1.024926	1.443093
C	-4.164216	-2.275879	3.805869
C	-3.062648	-0.413741	2.705298
C	-3.899179	-2.271757	1.390219
C	-4.351693	-2.890325	2.563441
C	-3.521663	-1.032695	3.874290
H	-2.601100	0.568476	2.769214
H	-4.062267	-2.756291	0.434524
H	-4.856785	-3.848407	2.501407
H	-3.390418	-0.540057	4.832497
H	-4.522209	-2.754276	4.711052
C	-3.419601	1.424080	-0.111814
C	-4.737178	3.908321	-0.323499
C	-4.503274	1.735602	0.733954
C	-3.016599	2.371450	-1.074616
C	-3.670413	3.602753	-1.176629
C	-5.152991	2.971299	0.627848
H	-4.851645	1.021466	1.469949
H	-2.203948	2.143296	-1.753228
H	-3.342539	4.319200	-1.922024
H	-5.986803	3.194508	1.285394
H	-5.243379	4.864486	-0.404035
C	-3.330253	-1.144542	-1.464238
C	-4.539860	-2.591484	-3.550795
C	-4.666290	-0.883542	-1.833858
C	-2.604350	-2.132615	-2.157033
C	-3.212993	-2.851384	-3.192505
C	-5.264939	-1.605262	-2.870414
H	-5.235322	-0.113742	-1.324596
H	-1.567800	-2.318300	-1.902042
H	-2.643397	-3.604761	-3.726661
H	-6.291447	-1.392209	-3.149503
H	-5.004657	-3.146368	-4.359062
C	3.436713	0.308849	1.571714
C	4.768472	1.022258	3.959003
C	2.726259	0.835538	2.666330
C	4.839270	0.185985	1.681126
C	5.494651	0.530253	2.866234
C	3.385021	1.186496	3.852199
H	1.666598	1.040964	2.573889
H	5.421677	-0.163767	0.835948
H	6.572455	0.426172	2.932319
H	2.820127	1.602920	4.679857
H	5.281278	1.292894	4.875656
C	3.219228	-1.702519	-0.585670

C	4.073359	-4.222375	-1.523404
C	2.850023	-2.154907	-1.870988
C	3.996177	-2.547417	0.231142
C	4.419010	-3.797498	-0.237181
C	3.284571	-3.399081	-2.336347
H	2.212830	-1.543599	-2.499298
H	4.276982	-2.241737	1.231488
H	5.020513	-4.432892	0.404488
H	3.002071	-3.724754	-3.332036
H	4.410383	-5.187058	-1.888026
C	3.374563	1.197074	-1.115777
C	4.526534	3.234388	-2.679245
C	3.216093	2.551451	-0.758062
C	4.125120	0.876643	-2.259638
C	4.697288	1.893342	-3.034441
C	3.785780	3.561400	-1.536246
H	2.661921	2.822507	0.134642
H	4.268646	-0.155496	-2.553435
H	5.274689	1.631848	-3.914955
H	3.649457	4.599147	-1.251980
H	4.967967	4.019126	-3.284212

Complex 2-Monomer (PBE1PBE; HF= -9763.0298729 a.u.**)**

Re	0.005558	-0.070892	0.027802
I	0.055972	0.555028	-2.661994
O	0.075536	-1.985969	-0.457005
N	-0.113238	1.542894	0.688347
C	-0.281431	2.776964	1.243728
C	-0.611032	5.342637	2.300856
C	-0.552231	2.953793	2.618892
C	-0.181466	3.913813	0.400563
C	-0.346850	5.189027	0.946453
C	-0.716504	4.224273	3.144554
H	-0.635108	2.075606	3.251491
H	-0.266184	6.040179	0.281615
H	-0.927248	4.354914	4.199344
H	-0.738611	6.338796	2.709331
O	0.072239	3.827783	-0.932316
H	0.193558	2.914547	-1.277335
N	0.039048	-1.118186	1.999291
H	0.655301	-0.610619	2.633539
H	-0.908021	-1.131858	2.392032
C	0.540362	-2.505323	1.796629
C	0.415421	-4.803087	2.589155
C	0.426503	-4.364687	0.182925
C	0.635338	-5.224725	1.199316
C	-0.114652	-3.005431	0.522800
C	0.331048	-3.495951	2.911723

H	0.351588	-5.565766	3.358565
H	0.551325	-4.631581	-0.859883
H	0.951966	-6.245126	1.012261
H	-1.202943	-3.111159	0.708444
H	0.224521	-3.156661	3.937786
H	1.617893	-2.412557	1.590683
P	2.530356	-0.048778	-0.017585
P	-2.506672	-0.244159	-0.077929
C	-3.174774	-1.058845	1.424521
C	-4.063264	-2.317298	3.780012
C	-3.011402	-0.435848	2.679276
C	-3.792036	-2.317743	1.371605
C	-4.231121	-2.940610	2.543137
C	-3.456692	-1.059982	3.846268
H	-2.578463	0.560937	2.734448
H	-3.938266	-2.806285	0.414003
H	-4.711387	-3.911381	2.484680
H	-3.343912	-0.559985	4.802827
H	-4.411508	-2.801274	4.685868
C	-3.363766	1.373324	-0.104381
C	-4.690383	3.841620	-0.294292
C	-4.467645	1.653905	0.718735
C	-2.945263	2.339031	-1.034377
C	-3.603581	3.564446	-1.125353
C	-5.122635	2.883264	0.622937
H	-4.826143	0.917893	1.429419
H	-2.115245	2.125980	-1.698273
H	-3.262323	4.299309	-1.846168
H	-5.974667	3.086236	1.263098
H	-5.201705	4.795578	-0.365952
C	-3.250948	-1.175163	-1.459022
C	-4.449740	-2.633626	-3.527501
C	-4.588005	-0.929291	-1.817527
C	-2.516100	-2.150889	-2.150953
C	-3.120723	-2.876436	-3.178958
C	-5.181970	-1.658047	-2.846681
H	-5.159984	-0.163263	-1.304270
H	-1.474791	-2.318775	-1.896020
H	-2.545911	-3.623266	-3.716230
H	-6.212113	-1.458230	-3.121250
H	-4.912426	-3.195293	-4.332085
C	3.357771	0.360440	1.567949
C	4.663751	1.137105	3.936165
C	2.637284	0.911704	2.638281
C	4.755982	0.247709	1.686334
C	5.398974	0.622939	2.864370
C	3.284152	1.294664	3.816148
H	1.577248	1.113480	2.526866

H	5.343370	-0.115301	0.849219
H	6.476711	0.527565	2.940923
H	5.168878	1.433190	4.849025
C	3.175892	-1.673061	-0.545595
C	4.054162	-4.183574	-1.451574
C	2.806856	-2.142276	-1.819957
C	3.963094	-2.493611	0.278548
C	4.397501	-3.741000	-0.174568
C	3.254835	-3.382933	-2.270615
H	2.156530	-1.543599	-2.449058
H	4.240553	-2.169893	1.275329
H	5.007642	-4.361981	0.472617
H	2.973729	-3.724566	-3.261175
H	4.402362	-5.148157	-1.805379
C	3.296206	1.199251	-1.114384
C	4.390323	3.227339	-2.709580
C	3.120054	2.549797	-0.768588
C	4.036751	0.874592	-2.257940
C	4.581070	1.888610	-3.049294
C	3.660657	3.556621	-1.564503
H	2.574825	2.818783	0.131485
H	4.192973	-0.160708	-2.537089
H	5.153005	1.626993	-3.933064
H	3.510017	4.595360	-1.292175
H	4.810007	4.011477	-3.330287

Complex 2-Dimer (B3LYP; HF=-19529.2881059 a.u.**)**

Re	-5.982860	0.093780	0.106635
I	-6.416673	-0.099177	2.887458
O	-3.961269	0.249247	0.462812
N	-7.587640	-0.054399	-0.618642
C	-8.641633	-0.184170	-1.444817
C	-10.853922	-0.514239	-3.144264
C	-9.965992	-0.239472	-0.908360
C	-8.413553	-0.281242	-2.891491
C	-9.594406	-0.459922	-3.697716
C	-11.054387	-0.400562	-1.737298
H	-10.086537	-0.136802	0.165165
H	-9.440439	-0.543745	-4.768030
H	-12.057791	-0.436664	-1.327398
H	-11.718287	-0.644354	-3.790193
O	-7.233534	-0.205622	-3.410414
H	-5.605523	-0.308518	-2.539539
N	-5.079142	0.327377	-1.910864
H	-5.342002	1.256025	-2.253206
C	-3.626843	0.201652	-1.872123
C	-1.418891	0.083485	-2.834293
C	-1.687903	0.133166	-0.412797

C	-0.866969	0.076186	-1.542990
C	-3.080671	0.196216	-0.577175
C	-2.808121	0.153226	-3.001453
H	-0.769717	0.039469	-3.701940
H	-1.273397	0.119705	0.588105
H	0.210397	0.027505	-1.419914
H	-3.249441	0.169909	-3.993691
P	-5.665954	-2.411835	0.030443
P	-6.195944	2.603030	0.288852
C	-5.604703	3.474947	-1.231513
C	-4.670077	4.657848	-3.619278
C	-6.287283	3.273242	-2.453672
C	-4.442024	4.268060	-1.232803
C	-3.981008	4.854887	-2.418102
C	-5.823906	3.864397	-3.634629
H	-7.181729	2.658051	-2.486618
H	-3.896491	4.428427	-0.310311
H	-3.082187	5.462841	-2.398986
H	-6.361556	3.696030	-4.561911
H	-4.309458	5.112570	-4.536261
C	-7.932609	3.210243	0.468770
C	-10.566518	4.140230	0.867866
C	-8.395875	4.365127	-0.192968
C	-8.810247	2.530055	1.335952
C	-10.113837	2.996472	1.534894
C	-9.704183	4.822639	0.003730
H	-7.743015	4.908340	-0.866006
H	-8.468748	1.647273	1.863529
H	-10.774058	2.461911	2.210572
H	-10.044580	5.711529	-0.518230
H	-11.580723	4.496025	1.019800
C	-5.286324	3.455090	1.649548
C	-3.855070	4.771599	3.684832
C	-5.759613	4.667806	2.187116
C	-4.090294	2.903324	2.149089
C	-3.380723	3.565635	3.157590
C	-5.047391	5.320391	3.198708
H	-6.686653	5.098605	1.826209
H	-3.733212	1.955028	1.762622
H	-2.463329	3.128248	3.538804
H	-5.427466	6.251162	3.608197
H	-3.305172	5.276749	4.472980
C	-5.850148	-3.114073	-1.670527
C	-6.161107	-4.033073	-4.320787
C	-7.034005	-3.760594	-2.072375
C	-4.823906	-2.933697	-2.621678
C	-4.978384	-3.393474	-3.932398
C	-7.186404	-4.213417	-3.388278

H	-7.840264	-3.910381	-1.364535
H	-3.900198	-2.440393	-2.340041
H	-4.175901	-3.247124	-4.648613
H	-8.109415	-4.704148	-3.680168
H	-6.282798	-4.382741	-5.341005
C	-4.031854	-3.038145	0.616261
C	-1.589355	-4.012261	1.637934
C	-3.444660	-2.447434	1.753130
C	-3.382149	-4.130579	0.007686
C	-2.168493	-4.609942	0.513579
C	-2.234781	-2.935812	2.256994
H	-3.929266	-1.609424	2.235936
H	-3.817177	-4.606981	-0.862753
H	-1.679454	-5.448447	0.027580
H	-1.797746	-2.468686	3.134210
H	-0.642925	-4.376849	2.024668
C	-6.875862	-3.405447	1.015950
C	-8.764810	-4.935837	2.444816
C	-6.501038	-4.614513	1.631465
C	-8.209264	-2.971039	1.135033
C	-9.147059	-3.735122	1.836778
C	-7.439400	-5.371366	2.342543
H	-5.477606	-4.964329	1.566448
H	-8.511725	-2.032669	0.690337
H	-10.170890	-3.384031	1.917173
H	-7.131033	-6.297520	2.817505
H	-9.491091	-5.523159	2.997944
Re	5.893257	-0.093134	-0.069636
I	3.421399	0.408766	-1.334763
O	6.714586	-0.489488	-1.920015
N	5.604133	0.226167	1.644280
C	5.704325	0.441860	2.967318
C	5.904318	0.953563	5.722023
C	4.537011	0.752771	3.733037
C	7.023322	0.365485	3.607600
C	7.048792	0.650629	5.019474
C	4.629905	1.004145	5.083838
H	3.580018	0.770932	3.221959
H	8.018308	0.609235	5.503742
H	3.742514	1.235258	5.662718
H	5.967317	1.157144	6.787682
O	8.090050	0.054257	2.949713
H	8.319678	0.034949	1.105025
N	8.008442	-0.617268	0.360673
H	8.006524	-1.523439	0.837982
C	8.808499	-0.695250	-0.855627
C	10.847398	-0.973644	-2.113429
C	8.716075	-0.765907	-3.280845

C	10.104400	-0.925474	-3.303899
C	8.059728	-0.650399	-2.044596
C	10.193544	-0.864165	-0.879041
H	11.924292	-1.098304	-2.146431
H	8.135360	-0.717783	-4.194178
H	10.614214	-1.010515	-4.258524
H	10.751258	-0.908256	0.051732
P	6.524793	2.330861	-0.456892
P	5.243818	-2.517942	0.189253
C	6.676044	-3.589296	0.664297
C	8.943699	-5.102031	1.400443
C	7.332176	-3.355994	1.895298
C	7.184891	-4.582957	-0.192520
C	8.308595	-5.333935	0.175862
C	8.454047	-4.109779	2.258734
H	6.969762	-2.588853	2.573290
H	6.704498	-4.772746	-1.145018
H	8.685127	-6.097689	-0.497091
H	8.943668	-3.913573	3.206857
H	9.814666	-5.684783	1.682440
C	4.022097	-2.839813	1.540341
C	2.080288	-3.313148	3.532251
C	4.146589	-3.932752	2.420897
C	2.904056	-1.992463	1.668397
C	1.941338	-2.231647	2.654297
C	3.184002	-4.163783	3.410858
H	4.994833	-4.602080	2.343179
H	2.782459	-1.155883	0.991142
H	1.084178	-1.570692	2.734032
H	3.300681	-5.006886	4.084552
H	1.338416	-3.489291	4.305050
C	4.526223	-3.382020	-1.272068
C	3.501275	-4.733903	-3.517392
C	3.651438	-4.474404	-1.110714
C	4.874983	-2.967220	-2.572131
C	4.365778	-3.646817	-3.684843
C	3.142934	-5.144645	-2.228006
H	3.358513	-4.796249	-0.117604
H	5.521656	-2.106923	-2.705564
H	4.636661	-3.315418	-4.682302
H	2.465388	-5.981438	-2.090073
H	3.103047	-5.253020	-4.383705
C	7.911018	2.896122	0.629119
C	10.021670	3.617705	2.358499
C	7.665187	3.670224	1.778884
C	9.234413	2.486324	0.362592
C	10.278759	2.848440	1.218037
C	8.713629	4.024568	2.636120

H	6.658605	3.997318	2.009946
H	9.453527	1.889834	-0.516009
H	11.290724	2.526027	0.993657
H	8.502737	4.617164	3.520530
H	10.832433	3.892739	3.025444
C	7.058137	2.762704	-2.169975
C	7.719638	3.469081	-4.818541
C	6.340246	2.222289	-3.256096
C	8.105128	3.668680	-2.431705
C	8.434410	4.015167	-3.747387
C	6.670794	2.576907	-4.567969
H	5.529608	1.529065	-3.073909
H	8.665620	4.105854	-1.614037
H	9.245540	4.713045	-3.930556
H	6.106658	2.152576	-5.392502
H	7.975465	3.738665	-5.838611
C	5.207456	3.580671	-0.106947
C	3.247727	5.510989	0.509406
C	5.175402	4.812378	-0.788188
C	4.239258	3.328803	0.882360
C	3.271417	4.290044	1.191839
C	4.200555	5.768387	-0.482447
H	5.903158	5.025900	-1.562246
H	4.233888	2.378944	1.399605
H	2.531153	4.077441	1.956403
H	4.185897	6.710143	-1.022108
H	2.490604	6.252626	0.743965

Complex 2-Dimer (PBE1PBE; HF= -19522.9443116 a.u.**)**

Re	-5.758650	-0.054622	-0.074593
I	-5.920169	0.617106	-2.764178
O	-3.800290	-0.565912	-0.387470
N	-7.326075	0.345438	0.611036
C	-8.365829	0.606339	1.415970
C	-10.519471	1.216647	3.091481
C	-9.595294	1.070668	0.866701
C	-8.209098	0.418588	2.854535
C	-9.350041	0.764928	3.653422
C	-10.657642	1.370652	1.685215
H	-9.670285	1.164320	-0.212069
H	-9.243817	0.645407	4.725925
H	-11.594954	1.718328	1.265850
H	-11.361913	1.460665	3.732905
O	-7.122406	-0.035882	3.373515
H	-5.563776	-0.204331	2.580121
N	-5.075744	-0.793272	1.868494
H	-5.493148	-1.717775	2.012119
C	-3.632546	-0.893051	1.929364

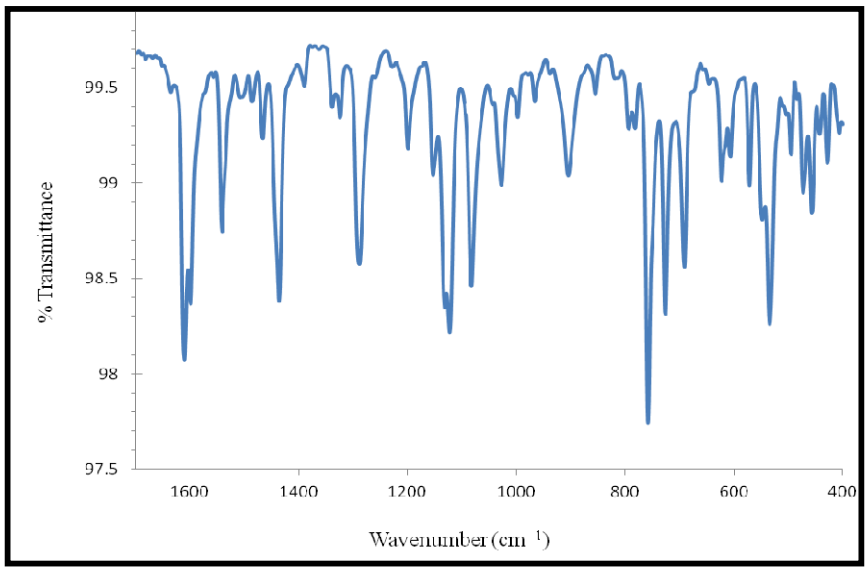
C	-1.512430	-1.237172	3.009790
C	-1.606755	-0.899629	0.604238
C	-0.873235	-1.118758	1.769329
C	-2.999259	-0.788140	0.683748
C	-2.903490	-1.131203	3.091054
H	-0.928593	-1.407190	3.907547
H	-1.120185	-0.787385	-0.357024
H	0.208993	-1.180349	1.712054
H	-3.416250	-1.223368	4.044088
P	-4.947472	2.228020	0.435820
P	-6.488806	-2.341690	-0.671876
C	-6.226018	-3.538437	0.696195
C	-5.763678	-5.231612	2.893432
C	-6.938526	-3.363198	1.900560
C	-5.273259	-4.565113	0.616672
C	-5.047493	-5.406431	1.708873
C	-6.708738	-4.207388	2.988047
H	-7.671444	-2.565450	1.990041
H	-4.709206	-4.706939	-0.298686
H	-4.308048	-6.196748	1.631334
H	-7.262754	-4.054388	3.908003
H	-5.583295	-5.884975	3.740667
C	-8.287218	-2.499862	-1.003673
C	-11.018574	-2.737605	-1.623094
C	-9.023675	-3.616340	-0.573250
C	-8.937737	-1.505940	-1.752573
C	-10.292622	-1.629087	-2.061134
C	-10.380858	-3.730759	-0.879270
H	-8.541322	-4.395492	0.006709
H	-8.377148	-0.647262	-2.106118
H	-10.779470	-0.854290	-2.644535
H	-10.936594	-4.596976	-0.534844
H	-12.073942	-2.827101	-1.859602
C	-5.694408	-3.161509	-2.102145
C	-4.415804	-4.463627	-4.228053
C	-6.367459	-4.152562	-2.833671
C	-4.378283	-2.818120	-2.450270
C	-3.745087	-3.474828	-3.506918
C	-5.728853	-4.799296	-3.892042
H	-7.391370	-4.411272	-2.585067
H	-3.871314	-2.028091	-1.903138
H	-2.729382	-3.201152	-3.773581
H	-6.259377	-5.559648	-4.456166
H	-3.921695	-4.965755	-5.053907
C	-5.185586	2.687504	2.196700
C	-5.642142	3.241838	4.914553
C	-6.260247	3.500557	2.588902
C	-4.342632	2.154677	3.188244

C	-4.568228	2.435295	4.534574
C	-6.486532	3.770968	3.939708
H	-6.924654	3.920494	1.842230
H	-3.507414	1.520503	2.909267
H	-3.906708	2.016606	5.286219
H	-7.327932	4.393543	4.225669
H	-5.821828	3.451383	5.963992
C	-3.182203	2.544888	0.076538
C	-0.504268	3.028187	-0.613526
C	-2.671038	2.090025	-1.151332
C	-2.341465	3.262002	0.943226
C	-1.007852	3.494411	0.600869
C	-1.341824	2.337020	-1.491092
H	-3.312439	1.537367	-1.828004
H	-2.721692	3.634181	1.887957
H	-0.359867	4.033415	1.284690
H	-0.955058	1.980570	-2.440075
H	0.536816	3.195518	-0.868983
C	-5.804161	3.592846	-0.442688
C	-7.159798	5.712974	-1.685405
C	-5.143418	4.802331	-0.705809
C	-7.148891	3.455788	-0.816050
C	-7.823560	4.512890	-1.427177
C	-5.818472	5.854446	-1.326021
H	-4.099966	4.919030	-0.433188
H	-7.659100	2.517078	-0.637883
H	-8.863791	4.392373	-1.711368
H	-5.294079	6.782405	-1.530286
H	-7.682938	6.531602	-2.169302
Re	5.665456	0.090530	0.006678
I	3.285507	-0.080746	1.423382
O	6.436784	1.156808	1.579777
N	5.419011	-0.833147	-1.468033
C	5.554416	-1.511339	-2.615391
C	5.843982	-2.992910	-4.969915
C	4.431205	-2.170892	-3.193579
C	6.869561	-1.576197	-3.246314
C	6.946079	-2.365145	-4.443108
C	4.567446	-2.898542	-4.350614
H	3.469116	-2.069871	-2.701712
H	7.919821	-2.434667	-4.915057
H	3.711306	-3.395384	-4.792553
H	5.944316	-3.574420	-5.882177
O	7.891856	-0.961026	-2.765354
H	8.039524	-0.241524	-1.159398
N	7.697533	0.590040	-0.628889
H	7.625191	1.309305	-1.354747
C	8.501814	1.082491	0.469318

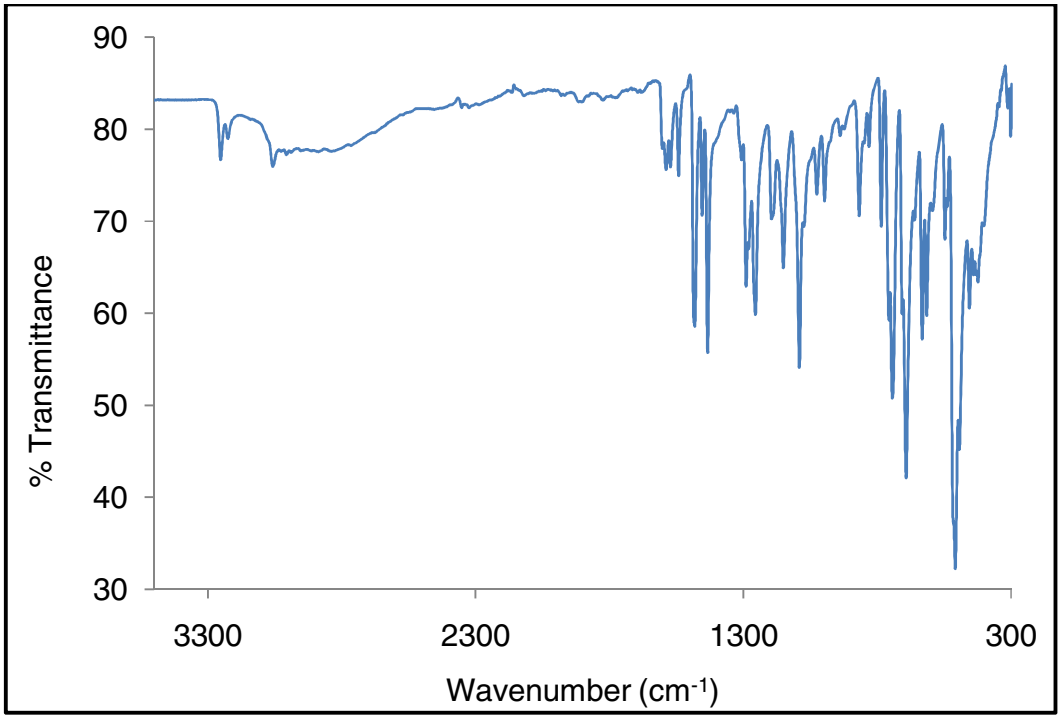
C	10.532375	1.824108	1.521377
C	8.427203	1.929583	2.736072
C	9.804546	2.135589	2.676268
C	7.768065	1.398525	1.621091
C	9.874861	1.299679	0.405454
H	11.603369	1.990815	1.489848
H	7.857091	2.156639	3.628774
H	10.319244	2.541108	3.541433
H	10.420362	1.058747	-0.502092
P	6.457169	-1.949394	1.155026
P	4.841716	2.173391	-1.044269
C	6.176699	3.097399	-1.902151
C	8.336894	4.375029	-3.168824
C	6.809722	2.503999	-3.013560
C	6.651539	4.330108	-1.429610
C	7.723520	4.964062	-2.062573
C	7.879490	3.142861	-3.642235
H	6.468146	1.542500	-3.388027
H	6.181561	4.793921	-0.569155
H	8.078224	5.918213	-1.686974
H	8.357064	2.670229	-4.493788
H	9.170255	4.869424	-3.656950
C	3.617327	1.901099	-2.384426
C	1.672758	1.492709	-4.371495
C	3.606856	2.690155	-3.547312
C	2.639041	0.906586	-2.229163
C	1.674036	0.707188	-3.217374
C	2.640211	2.485456	-4.533082
H	4.358956	3.458936	-3.688849
H	2.629468	0.301691	-1.329017
H	0.923830	-0.065668	-3.083348
H	2.646850	3.100411	-5.427133
H	0.924506	1.331043	-5.140707
C	4.070780	3.444545	0.024546
C	2.954317	5.423678	1.666299
C	3.188210	4.396753	-0.511151
C	4.386821	3.488526	1.391572
C	3.830264	4.479384	2.202962
C	2.633019	5.381091	0.307329
H	2.927811	4.366830	-1.564380
H	5.056004	2.742136	1.809809
H	4.075664	4.503504	3.259644
H	1.948424	6.109217	-0.115855
H	2.520636	6.188616	2.302713
C	7.835266	-2.760043	0.255225
C	9.918548	-3.877903	-1.264651
C	7.595219	-3.856727	-0.586878
C	9.136071	-2.229692	0.323524

C	10.168187	-2.789035	-0.427654
C	8.631518	-4.407599	-1.342913
H	6.599500	-4.280274	-0.657595
H	9.344556	-1.379405	0.965004
H	11.166608	-2.368627	-0.361727
H	8.426236	-5.249061	-1.996285
H	10.721590	-4.306369	-1.855300
C	7.059300	-1.740637	2.872050
C	7.832693	-1.470433	5.559002
C	6.331599	-0.910926	3.742273
C	8.171281	-2.440734	3.368956
C	8.556194	-2.301817	4.703596
C	6.718968	-0.781288	5.075956
H	5.469334	-0.368668	3.373492
H	8.737768	-3.096544	2.717147
H	9.418982	-2.847423	5.072058
H	6.146514	-0.138325	5.736724
H	8.132634	-1.363342	6.596635
C	5.231856	-3.308885	1.310485
C	3.416637	-5.444514	1.480156
C	5.323432	-4.240118	2.356347
C	4.215132	-3.457072	0.355951
C	3.318099	-4.522365	0.437551
C	4.419234	-5.299619	2.440186
H	6.094293	-4.133723	3.111795
H	4.118476	-2.729668	-0.440059
H	2.535316	-4.622285	-0.307125
H	4.497489	-6.007967	3.258591
H	2.712208	-6.267232	1.548108

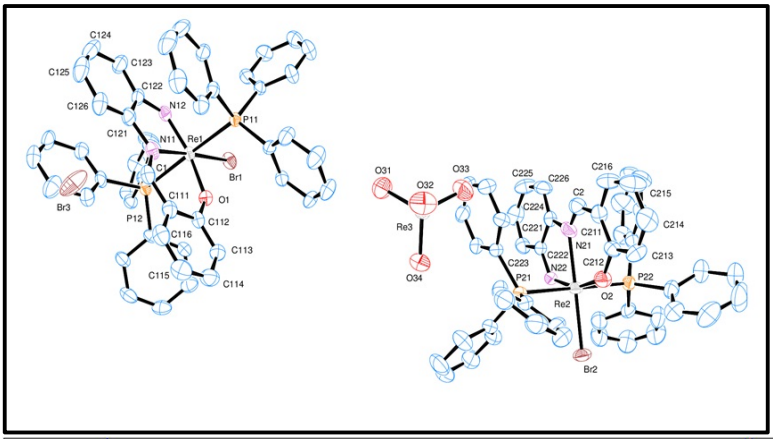
6. **IR of complex 1**

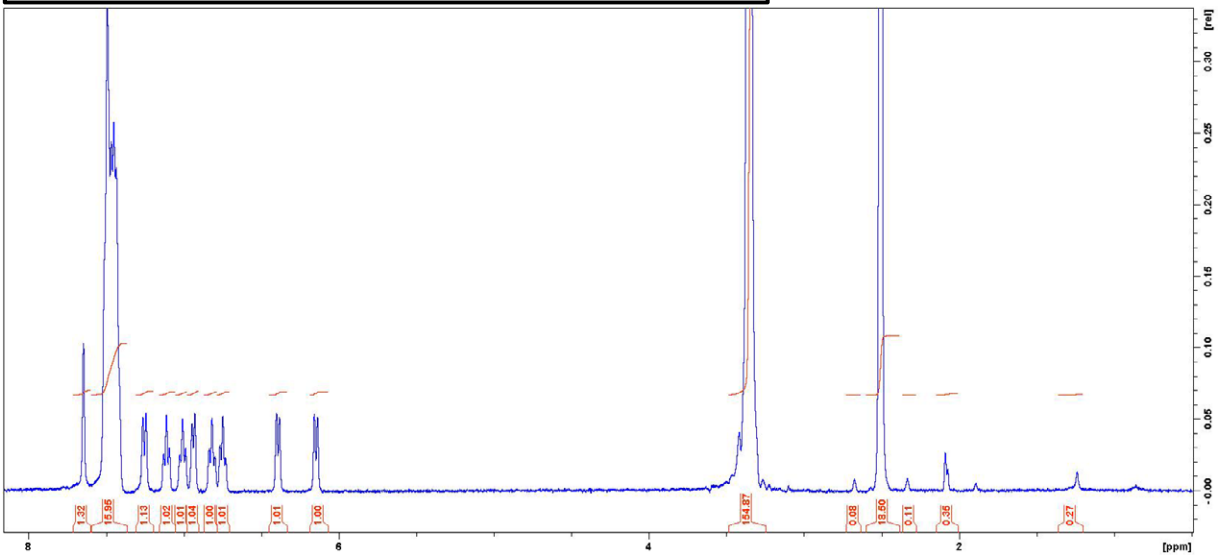


7. IR of complex **2**



8. ^{1}NMR of complex **1**





9. ^{1}NMR of complex **2**