Supporting Information

Ligand-Modulated Metallophilicity: Influence of π-Acceptor and σ-Donor Strength

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Computational details

Geometry optimization

The dimers of **Rh-1**, **Rh-2**, **Rh-3**, **Rh-4**, **Au-1**, **Au-2**, **Pt-1**, and **Pt-2** extracted directly from the X-ray crystal structures were employed as the initial geometry for optimization.[1-8] For **Rh(terpy)L** dimers, the initial structures were derived from the X-ray crystal structure of **Rh-2** dimer by replacing its two acetonitrile (ACN) ligands with target ligands L (L = [NH_3, PH_3, CO, $CNCH_3$, $CCCH_3$, CN, Cl, Br, I]). The ligand conformations and Rh-L bond distances were set to default values in GaussView 6[9] prior to optimization.

All geometry optimizations were performed using Gaussian 16[10], with the hybrid PBE0 functional[11] and D3 version of Grimme's dispersion with Becke-Johnson damping[12,13].The basis sets of 6-31G(d)[14,15] were used for light elements (H, C, N, O, P, S, Cl, Br). The Stuttgart/Dresden effective core potential (SDD) with its associated basis sets[16,17] were employed for heavy atoms (I, Rh, Pt, Au) to account for scalar relativistic effects. All geometry optimizations were performed in ACN solvent, modeled using the integral equation formalism polarizable continuum model (IEF-PCM) with Gaussian 16's default parameters for ACN (dielectric constant $\varepsilon = 35.688$).[18] All optimized structures were verified as local minima (no imaginary frequencies) at the same theory level.

Energy decomposition analysis (EDA) and natural orbitals for chemical valence (NOCV)

The metal–metal (M–M) Pauli repulsion was calculated using EDA[19,20] following the previously reported method.[21,22] All EDA calculations were based on the above-mentioned optimized complex dimers, with fragment geometries frozen when changing M–M distances. The relative π-accepting and σ-donating abilities of the ligands were analyzed using NOCV method.[23] The complex monomers used for NOCV calculations were extracted directly from the optimized dimers without further optimization, and each monomer was partitioned into two fragments: the target ligand fragment and the remaining part.

All EDA and NOCV calculations were performed using the Amsterdam Modeling Suite (AMS) 2024.1 software package.[24,25] Hybrid functional PBE0 and D3BJ dispersion corrections were used for all calculations. Scalar relativistic effects were treated via zeroth order regular approximation (ZORA).[26-28] The all-electron ZORA/TZ2P basis sets were applied to all elements, utilizing triple-ζ Slater-type orbitals (STO) for valence orbitals augmented with two polarization functions (p- and d- functions for H; d- and f-functions for C, N, O, P, S, Cl, Br, and I; p- and f-functions for Rh, Pt, and Au).[29] The figures of molecular orbitals and NOCV isosurfaces were generated with AMSview 2024.

Molecular volume

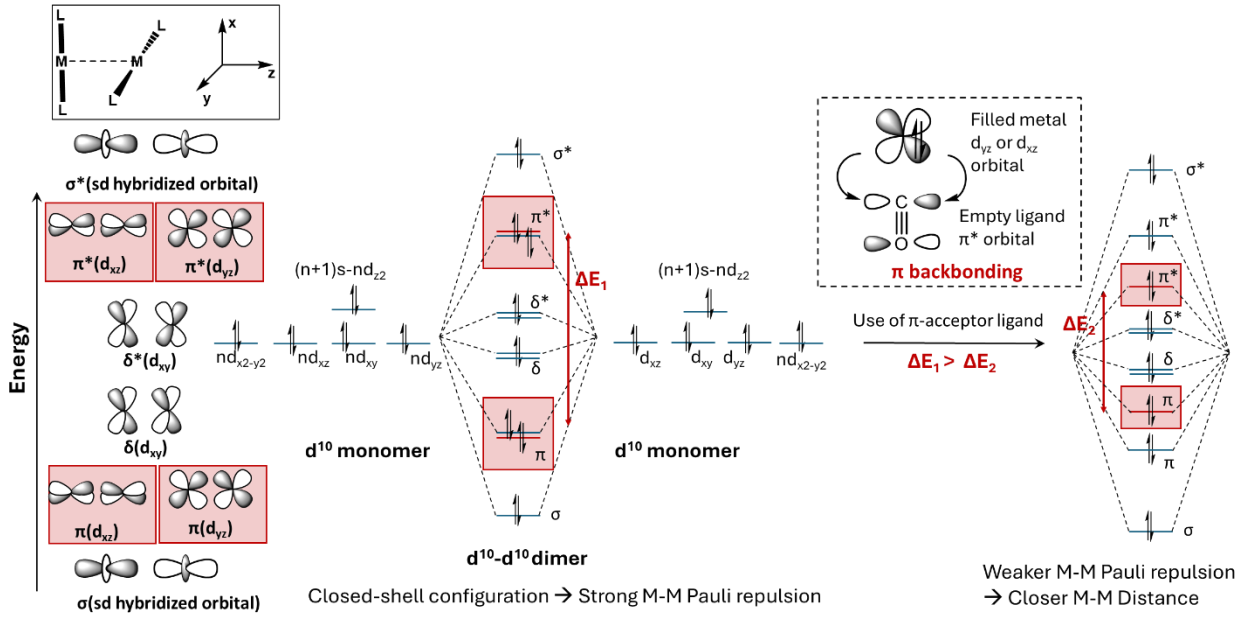
The molecular volumes of **Rh(terpy)L** complexes were calculated using Multiwfn 3.8 (dev version).[30,31] Wavefunction files were generated from monomers extracted from optimized dimers at the

same theoretical level via single-point calculations. The Monte Carlo method employed 819,200 points, using the 0.001 e/Bohr^3 electron density isosurface as the molecular boundary.

Local energy decomposition (LED)

The relative magnitude of M–M Pauli repulsion in **Rh-1** and **Rh-2** dimers was validated using local energy decomposition (LED)[32] based on domain-based local pair natural orbital coupled cluster with singles, doubles, and perturbative triples (DLPNO-CCSD(T)) calculations.[33,34] All calculations were based on the above-mentioned optimized **Rh-1** and **Rh-2** dimers, with fragment geometries frozen when changing M–M distances. LED calculations were performed in ORCA 6.0[35] following the previously reported method.[21,22] The Ahlrichs basis sets of def2-TZVP[36] were used for light elements (H, C, N, Cl) and the def2-TZVP basis set was combined with the effective core potential (def2-ECP) for Rh to account for relativistic effects. The evaluation of two-electron integrals in DLPNO-CCSD(T) calculations was accelerated using the density-fitting approximation with the JK auxiliary basis (RI-JK).[37,38] Tight PNO was used for calculations.

Figures



Scheme S1. Illustration scheme to show the role of π-acceptor ligand in weakening the M–M Pauli repulsion for d^{10}-d^{10} closed-shell metal complexes, by forming the π-backbonding interaction between the ligand and metal atom.

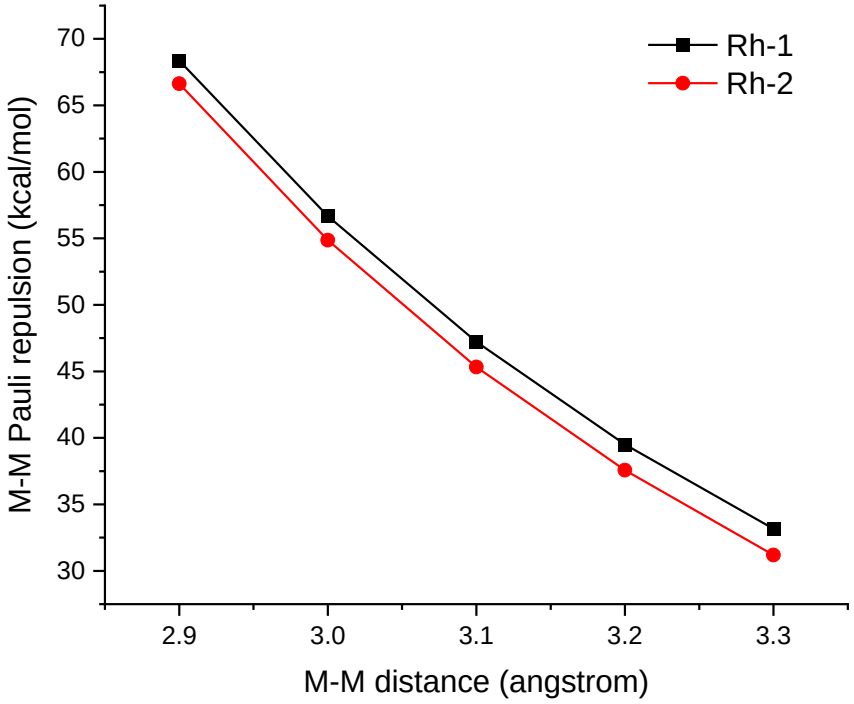


Figure S1. Calculated Rh–Rh Pauli repulsion in the [**Rh-1**]$_2$ and [**Rh-2**]$_2$ dimers as a function of metal–metal distance, in the framework of the DLPNO-CCSD(T) method.

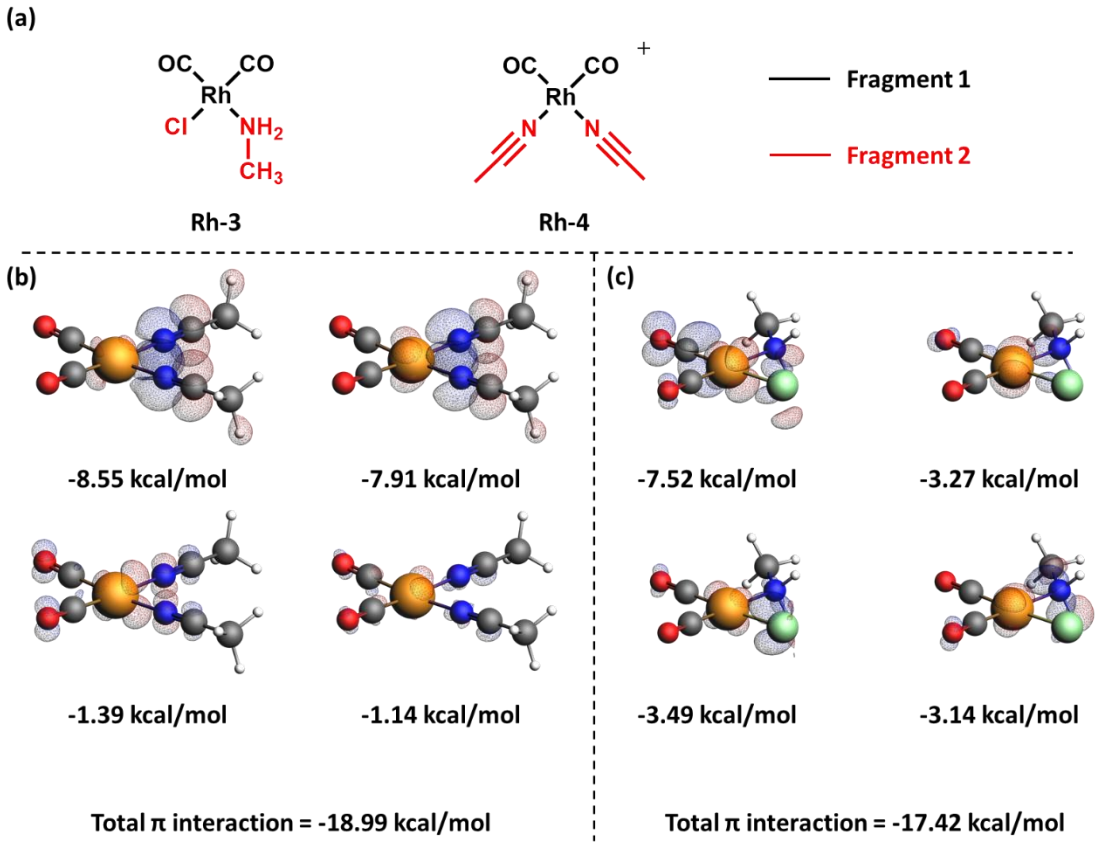
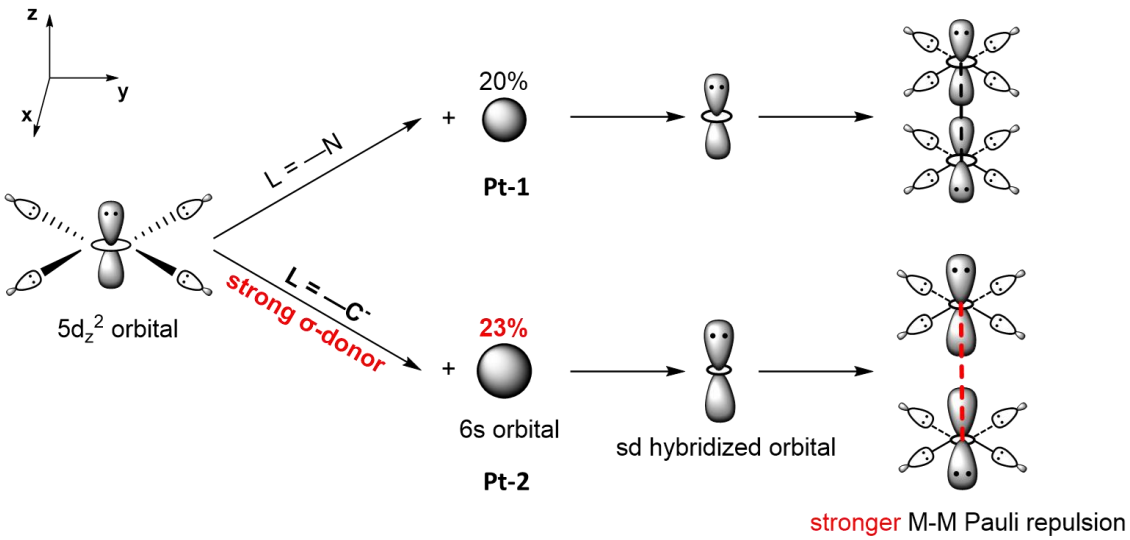


Figure S2. (a) Chemical structures and fragmentation used for NOCV analysis of **Rh-3** and **Rh-4**. Calculated EDA-NOCV deformation density contributions to π-backbonding in (b) **Rh-4** and (c) **Rh-3**, together with the calculated orbital energies. Isovalue = 0.001. Charge transfer from red to blue.

Table S1. Key parameters for **Rh(terpy)L**: M–M distance of optimized dimers, M–M Pauli repulsion and L–L dispersion at fixed M–M distance (3.1 Å) of dimers, molecular volume of monomers, and energies of M→L π interaction via NOCV.

Ligand	M–M distance (Å)	M–M Pauli repulsion (kcal/mol)	L-L dispersion (kcal/mol)	Molecular volume ($Å^3$)	Energy of M→L π interaction (kcal/mol)
CO	3.00855	19.04	-14.95	325.51	-27.21
$CNCH_3$	3.00935	21.47	-17.85	355.34	-16.25
$NCCH_3$	3.01057	22.57	-17.42	356.00	-8.99
PH_3	3.02281	19.31	-16.84	342.45	-10.52
^-CN	3.03588	23.94	-15.26	336.49	-5.04
NH_3	3.07443	24.79	-15.41	325.44	-1.83
$^-CCCH_3$	3.15568	25.47	-19.24	367.02	-6.68
Br^-	3.15736	24.03	-16.55	342.13	-2.40
I^-	3.22272	23.50	-14.41	356.77	-2.17
Cl^-	3.24436	24.75	-16.09	335.23	-2.34



Scheme S2. Illustration scheme to show the role of σ-donor ligand in strengthening the M–M Pauli repulsion for d^8-d^8 closed-shell metal complexes.

Cartesian coordinates of Gaussian outputs

Rh-1 dimer ($d_{Rh–Rh}$=4.98 Å)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.879205	1.582744	0.488595
2	17	0	-2.813819	3.470889	-0.644608
3	7	0	-0.034926	2.326019	0.944782
4	6	0	0.734764	1.455571	1.664794
5	6	0	2.035020	1.779912	2.036723
6	1	0	2.632786	1.070189	2.597628
7	6	0	2.563443	3.012632	1.671549
8	1	0	3.578454	3.275263	1.950486
9	6	0	1.774769	3.891723	0.936640
10	1	0	2.147397	4.861429	0.625282
11	6	0	0.484683	3.509487	0.593144
12	1	0	-0.175030	4.150258	0.018097
13	7	0	-1.171132	0.100396	1.478604
14	6	0	0.077500	0.187029	1.991533
15	6	0	0.596086	-0.861441	2.744425
16	1	0	1.595334	-0.800117	3.159609
17	6	0	-0.186605	-1.993289	2.956396
18	1	0	0.204073	-2.820307	3.538915
19	6	0	-1.463798	-2.069883	2.407302
20	1	0	-2.075270	-2.951513	2.562804
21	6	0	-1.943195	-0.997526	1.661523
22	7	0	-3.457753	0.302684	0.359629
23	6	0	-3.249507	-0.881690	1.008555
24	6	0	-4.215137	-1.883342	1.009254
25	1	0	-4.029742	-2.815203	1.531286
26	6	0	-5.407649	-1.685188	0.324647
27	1	0	-6.166746	-2.460439	0.312985
28	6	0	-5.604373	-0.483455	-0.349202
29	1	0	-6.516405	-0.287356	-0.902263
30	6	0	-4.608782	0.482651	-0.303539
31	1	0	-4.708439	1.441760	-0.800662
32	45	0	1.795020	-1.632630	-0.517056
33	17	0	2.490458	-3.678090	0.509745
34	7	0	-0.096027	-2.153269	-1.076247
35	6	0	-0.744006	-1.170515	-1.768431

36	6	0	-2.047014	-1.347540	-2.223925
37	1	0	-2.544672	-0.551502	-2.765814
38	6	0	-2.704328	-2.543699	-1.967390
39	1	0	-3.722751	-2.691599	-2.310668
40	6	0	-2.041079	-3.536139	-1.250877
41	1	0	-2.519222	-4.481578	-1.019439
42	6	0	-0.742292	-3.300796	-0.823253
43	1	0	-0.173952	-4.035069	-0.262521
44	7	0	1.275306	-0.026355	-1.426425
45	6	0	0.044351	0.046955	-1.981440
46	6	0	-0.340426	1.190781	-2.674515
47	1	0	-1.326305	1.260217	-3.118628
48	6	0	0.559056	2.246584	-2.788122
49	1	0	0.274250	3.145134	-3.324525
50	6	0	1.819526	2.155229	-2.202371
51	1	0	2.521908	2.976775	-2.283221
52	6	0	2.161604	0.995304	-1.515513
53	7	0	3.490025	-0.532442	-0.258052
54	6	0	3.426185	0.704433	-0.835283
55	6	0	4.488441	1.598783	-0.743888
56	1	0	4.417356	2.575226	-1.209724
57	6	0	5.629825	1.236090	-0.040247
58	1	0	6.463089	1.926093	0.043142
59	6	0	5.681303	-0.020279	0.556985
60	1	0	6.550184	-0.344000	1.119434
61	6	0	4.595040	-0.873133	0.421130
62	1	0	4.580258	-1.867065	0.855537

Rh-1 dimer ($d_{Rh–Rh}$=3.24 Å, used in subsequent computations)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.062895	-0.829132	1.392862
2	7	0	-1.934626	-1.202157	1.259285
3	7	0	0.108808	-2.448559	0.370044
4	7	0	2.077672	-1.071056	1.232179
5	17	0	0.013698	1.041327	2.896325
6	6	0	-2.940914	-0.478926	1.770347
7	6	0	-2.228150	-2.320460	0.530985
8	6	0	-1.058191	-3.038893	0.020400
9	6	0	1.306913	-2.960324	0.002277
10	6	0	2.434300	-2.167111	0.497656
11	6	0	3.040979	-0.284657	1.732574
12	1	0	-2.638270	0.399812	2.329649
13	6	0	-4.272393	-0.829107	1.601124
14	6	0	-3.545371	-2.720296	0.323879
15	6	0	-1.048315	-4.205802	-0.735847
16	6	0	1.363060	-4.125652	-0.754499
17	6	0	3.772125	-2.478546	0.271631
18	6	0	4.390210	-0.546492	1.545155
19	1	0	2.688744	0.571827	2.297426
20	1	0	-5.048917	-0.208751	2.034581
21	6	0	-4.580913	-1.970984	0.866603
22	1	0	-3.756990	-3.610645	-0.257727
23	1	0	-1.977118	-4.687271	-1.020556
24	6	0	0.173852	-4.748144	-1.125407
25	1	0	2.317410	-4.544579	-1.053188
26	1	0	4.034362	-3.351605	-0.315610
27	6	0	4.763345	-1.663752	0.802904
28	1	0	5.129844	0.122620	1.970630
29	1	0	-5.612245	-2.271107	0.712685
30	1	0	0.199560	-5.657361	-1.716346
31	1	0	5.810061	-1.894751	0.634259
32	45	0	-0.062929	0.829129	-1.392858
33	7	0	1.934606	1.202094	-1.259340
34	7	0	-0.108761	2.448558	-0.370040
35	7	0	-2.077693	1.071117	-1.232122
36	17	0	-0.013833	-1.041338	-2.896314
37	6	0	2.940858	0.478837	-1.770440

38	6	0	2.228188	2.320384	-0.531045
39	6	0	1.058265	3.038853	-0.020425
40	6	0	-1.306840	2.960362	-0.002241
41	6	0	-2.434267	2.167189	-0.497598
42	6	0	-3.041039	0.284751	-1.732493
43	1	0	2.638169	-0.399889	-2.329737
44	6	0	4.272352	0.828979	-1.601260
45	6	0	3.545427	2.720181	-0.323980
46	6	0	1.048447	4.205758	0.735828
47	6	0	-1.362930	4.125687	0.754543
48	6	0	-3.772075	2.478678	-0.271552
49	6	0	-4.390258	0.546639	-1.545051
50	1	0	-2.688847	-0.571750	-2.297345
51	1	0	5.048843	0.208603	-2.034748
52	6	0	4.580930	1.970842	-0.866742
53	1	0	3.757091	3.610522	0.257620
54	1	0	1.977274	4.687195	1.020516
55	6	0	-0.173692	4.748138	1.125424
56	1	0	-2.317259	4.544643	1.053259
57	1	0	-4.034268	3.351750	0.315689
58	6	0	-4.763336	1.663919	-0.802802
59	1	0	-5.129925	-0.122449	-1.970505
60	1	0	5.612275	2.270936	-0.712860
61	1	0	-0.199354	5.657352	1.716369
62	1	0	-5.810040	1.894958	-0.634138

Rh-2 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.001756	-0.320158	1.470839
2	7	0	-2.011462	-0.674007	1.469931
3	7	0	-0.003243	-2.194502	1.004445
4	7	0	2.007379	-0.677636	1.471457
5	7	0	-0.000295	1.562069	2.163830
6	6	0	-2.996459	0.183195	1.768652
7	6	0	-2.336004	-1.947387	1.097038
8	6	0	-1.187498	-2.813106	0.809488
9	6	0	1.180044	-2.815265	0.810502
10	6	0	2.329891	-1.951638	1.098991
11	6	0	2.993683	0.177824	1.770841
12	6	0	0.000634	2.624910	2.623117
13	6	0	-4.336806	-0.172791	1.721235
14	1	0	-2.682975	1.181471	2.051665
15	6	0	-3.661385	-2.362396	1.024813
16	6	0	-1.213723	-4.137949	0.385765
17	6	0	1.204233	-4.140141	0.386760
18	6	0	3.654573	-2.369119	1.028019
19	6	0	4.333420	-0.180613	1.724620
20	1	0	2.681799	1.176740	2.053379
21	6	0	0.001763	3.942162	3.225634
22	6	0	-4.675923	-1.467749	1.341947
23	1	0	-5.094470	0.560442	1.973142
24	1	0	-3.897526	-3.377467	0.726480
25	6	0	-0.005253	-4.797843	0.172960
26	1	0	-2.154296	-4.650632	0.220784
27	1	0	2.143999	-4.654514	0.222484
28	6	0	4.670479	-1.476270	1.345885
29	1	0	3.889122	-3.384682	0.730098
30	1	0	5.092203	0.551290	1.977027
31	1	0	0.000561	3.849170	4.315756
32	1	0	0.893121	4.493737	2.914218
33	1	0	-0.887553	4.496057	2.912502
34	1	0	-5.714175	-1.777838	1.290680
35	1	0	-0.006056	-5.830198	-0.159936
36	1	0	5.708203	-1.788280	1.295603
37	1	0	0.888030	-4.495842	-2.911999

38	6	0	-0.001660	-3.942426	-3.224924
39	6	0	-0.000818	-2.625023	-2.622737
40	1	0	-0.000997	-3.849696	-4.315065
41	1	0	-0.892633	-4.494332	-2.912983
42	7	0	-0.000009	-1.562163	-2.163494
43	45	0	0.001596	0.320116	-1.470665
44	7	0	2.011375	0.673771	-1.470147
45	7	0	0.003361	2.194478	-1.004362
46	7	0	-2.007481	0.677923	-1.471312
47	6	0	2.996235	-0.183513	-1.769073
48	6	0	2.336093	1.947171	-1.097469
49	6	0	1.187707	2.812912	-0.809471
50	6	0	-1.179830	2.815343	-0.810146
51	6	0	-2.329828	1.951954	-1.098800
52	6	0	-2.993884	-0.177328	-1.770986
53	6	0	4.336612	0.172441	-1.722187
54	1	0	2.682630	-1.181838	-2.051782
55	6	0	3.661506	2.362182	-1.025896
56	6	0	1.214150	4.137625	-0.385333
57	6	0	-1.203811	4.140120	-0.386095
58	6	0	-3.654447	2.369660	-1.028025
59	6	0	-4.333559	0.181358	-1.725014
60	1	0	-2.682117	-1.176268	-2.053580
61	6	0	4.675904	1.467465	-1.343298
62	1	0	5.094155	-0.560871	-1.974233
63	1	0	3.897778	3.377314	-0.727879
64	6	0	0.005784	4.797605	-0.172205
65	1	0	2.154807	4.650098	-0.220207
66	1	0	-2.143495	4.654579	-0.221619
67	6	0	-4.670454	1.477036	-1.346190
68	1	0	-3.888857	3.385240	-0.730043
69	1	0	-5.092436	-0.550356	-1.977685
70	1	0	5.714180	1.777553	-1.292515
71	1	0	0.006732	5.829866	0.160984
72	1	0	-5.708132	1.789226	-1.296070

Rh-3 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.563786	3.322248	-0.535267
2	1	0	-0.253993	3.211646	0.179258
3	1	0	0.260458	4.031084	-1.311382
4	1	0	1.439819	3.712753	-0.014364
5	7	0	0.882126	2.008818	-1.117737
6	1	0	1.599597	2.117537	-1.834326
7	1	0	0.055150	1.646209	-1.603485
8	45	0	1.558852	0.367696	0.053591
9	6	0	1.232967	1.226705	1.649297
10	6	0	2.272309	-1.105726	0.926516
11	17	0	2.053006	-0.647907	-2.046524
12	8	0	1.022064	1.762349	2.643717
13	8	0	2.727884	-2.029585	1.430678
14	1	0	-0.054179	-1.645153	-1.603842
15	7	0	-0.881391	-2.008309	-1.118955
16	6	0	-0.563164	-3.322035	-0.537074
17	1	0	-1.598293	-2.116777	-1.836154
18	45	0	-1.558990	-0.367745	0.052777
19	1	0	0.254118	-3.211719	0.178056
20	1	0	-0.259183	-4.030317	-1.313434
21	1	0	-1.439468	-3.713044	-0.017004
22	6	0	-1.234359	-1.227602	1.648266
23	6	0	-2.272965	1.105333	0.925872
24	17	0	-2.051299	0.648983	-2.047205
25	8	0	-1.024123	-1.763825	2.642514
26	8	0	-2.728754	2.029138	1.429934

Rh-4 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.764745	-0.027838	1.364095
2	6	0	-0.374933	1.196511	2.177129
3	6	0	-0.205295	-1.442936	2.081625
4	7	0	2.129094	-1.347104	0.571851
5	7	0	1.944892	1.504856	0.666121
6	8	0	-1.052023	1.970057	2.675386
7	8	0	-0.775850	-2.332495	2.515232
8	6	0	2.912218	-2.069213	0.130228
9	6	0	2.626435	2.349201	0.275882
10	6	0	3.882706	-2.973622	-0.440403
11	6	0	3.472138	3.405694	-0.228204
12	1	0	3.618293	-3.175902	-1.482497
13	1	0	3.885418	-3.910838	0.122711
14	1	0	4.876691	-2.520090	-0.399416
15	1	0	4.129571	3.761166	0.570063
16	1	0	2.849983	4.232799	-0.581418
17	1	0	4.077221	3.025126	-1.055669
18	8	0	1.052571	-1.964595	-2.681663
19	6	0	0.376062	-1.192576	-2.180217
20	45	0	-0.763957	0.029395	-1.363953
21	6	0	0.204518	1.446457	-2.079705
22	7	0	-2.130444	1.345466	-0.570158
23	7	0	-1.942432	-1.505455	-0.667542
24	8	0	0.774258	2.337106	-2.512185
25	6	0	-2.916210	2.063577	-0.126690
26	6	0	-2.623051	-2.351084	-0.278457
27	6	0	-3.890879	2.962417	0.445569
28	6	0	-3.467434	-3.408874	0.225030
29	1	0	-3.595187	3.211801	1.468956
30	1	0	-3.940912	3.877022	-0.151425
31	1	0	-4.872057	2.480175	0.458242
32	1	0	-4.125162	-3.764002	-0.573157
33	1	0	-2.844309	-4.235712	0.576949
34	1	0	-4.072093	-3.029815	1.053505

Au-1 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.546018	-0.019196	0.151414
2	16	0	-1.828610	-1.696318	1.759192
3	16	0	-1.478904	1.640006	-1.503186
4	6	0	-0.281424	-1.846500	2.400366
5	6	0	-1.506843	3.020066	-0.539050
6	7	0	0.774234	-1.992648	2.884633
7	7	0	-1.524517	4.004835	0.092671
8	79	0	1.495136	-0.324508	-0.150738
9	16	0	1.790862	1.282303	1.531260
10	16	0	1.409799	-2.000063	-1.783347
11	6	0	2.196373	2.616765	0.588442
12	6	0	-0.115019	-1.774129	-2.454863
13	7	0	2.482180	3.568773	-0.028883
14	7	0	-1.164643	-1.660892	-2.960633

Au-2 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.000000	0.000000	1.611608
2	6	0	1.983179	0.181643	1.649177
3	6	0	-1.983179	-0.181643	1.649177
4	7	0	3.146694	0.288727	1.667904
5	7	0	-3.146694	-0.288727	1.667904
6	79	0	-0.000000	-0.000000	-1.612609
7	6	0	-0.000000	1.991531	-1.648116
8	6	0	0.000000	-1.991531	-1.648116
9	7	0	0.001044	3.160000	-1.663161
10	7	0	-0.001044	-3.160000	-1.663161

Pt-1 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	0.106043	0.220954	-1.588796
2	7	0	-0.964180	-1.507912	-1.678140
3	7	0	-1.730378	0.966810	-1.647066
4	7	0	0.544674	2.208797	-1.576762
5	6	0	1.922079	-0.513952	-1.559501
6	6	0	-0.472396	-2.749535	-1.675985
7	6	0	-2.316545	-1.306471	-1.718728
8	6	0	-2.753235	0.101194	-1.693952
9	6	0	-1.862479	2.301471	-1.635381
10	6	0	-0.567399	3.007984	-1.603570
11	6	0	1.763791	2.757528	-1.551416
12	6	0	3.055973	-0.978201	-1.493880
13	1	0	0.608322	-2.825816	-1.640036
14	6	0	-1.301547	-3.864377	-1.714444
15	6	0	-3.187887	-2.382966	-1.777044
16	6	0	-4.052534	0.599067	-1.719507
17	6	0	-3.140895	2.850351	-1.653620
18	6	0	-0.439440	4.388939	-1.603282
19	6	0	1.946048	4.134832	-1.546171
20	1	0	2.591681	2.057744	-1.532934
21	6	0	4.357992	-1.527637	-1.326173
22	1	0	-0.862298	-4.855186	-1.703399
23	6	0	-2.675930	-3.677659	-1.769309
24	1	0	-4.257866	-2.216401	-1.809614
25	1	0	-4.907850	-0.064505	-1.751089
26	6	0	-4.230807	1.981505	-1.692157
27	1	0	-3.293602	3.922920	-1.638962
28	1	0	-1.323138	5.015534	-1.623681
29	6	0	0.830126	4.960585	-1.573445
30	1	0	2.951258	4.539127	-1.520557
31	6	0	4.557530	-2.919975	-1.359483
32	6	0	5.459938	-0.693417	-1.065376
33	1	0	-3.350460	-4.526530	-1.799458
34	1	0	-5.235681	2.389213	-1.704784
35	1	0	0.938714	6.039681	-1.569067
36	1	0	3.710102	-3.569479	-1.558414
37	6	0	5.816470	-3.457589	-1.122284

38	6	0	6.716455	-1.238658	-0.825800
39	1	0	5.314130	0.382703	-1.046215
40	1	0	5.953611	-4.535033	-1.145596
41	6	0	6.898928	-2.620936	-0.848864
42	1	0	7.556723	-0.581577	-0.619791
43	1	0	7.880779	-3.044446	-0.658459
44	1	0	4.322573	-2.313233	1.681896
45	6	0	3.256680	-2.504472	1.648619
46	6	0	2.776154	-3.809486	1.579542
47	6	0	2.359170	-1.448105	1.652874
48	6	0	1.406363	-4.026992	1.526015
49	1	0	3.471448	-4.641829	1.561797
50	7	0	1.011554	-1.680513	1.607609
51	6	0	2.762036	-0.030978	1.700959
52	6	0	0.550083	-2.932358	1.546609
53	1	0	0.991025	-5.026497	1.469358
54	78	0	-0.098992	0.025395	1.603973
55	7	0	1.719247	0.811317	1.698496
56	6	0	4.049434	0.495137	1.748579
57	1	0	-0.528575	-3.033509	1.511363
58	7	0	-0.584253	2.001020	1.684497
59	6	0	-1.901911	-0.738167	1.531610
60	6	0	1.820060	2.147777	1.744730
61	1	0	4.920041	-0.148844	1.750108
62	6	0	4.195450	1.881171	1.779359
63	6	0	0.508459	2.824251	1.751301
64	6	0	-1.816366	2.519916	1.690420
65	6	0	-3.037490	-1.192836	1.436295
66	6	0	3.085571	2.725306	1.779000
67	1	0	5.190738	2.311158	1.806444
68	6	0	0.346878	4.199665	1.826237
69	6	0	-2.032190	3.890713	1.760157
70	1	0	-2.626644	1.801428	1.634895
71	6	0	-4.346554	-1.711579	1.230135
72	1	0	3.213576	3.800799	1.804908
73	1	0	1.214801	4.846007	1.881169
74	6	0	-0.936583	4.740665	1.829920
75	1	0	-3.047016	4.271164	1.757803
76	6	0	-4.569497	-3.099312	1.171049
77	6	0	-5.433357	-0.843116	1.022318
78	1	0	-1.071474	5.815383	1.885046
79	1	0	-3.733968	-3.774912	1.329060
80	6	0	-5.836803	-3.598416	0.896817

81	6	0	-6.698338	-1.349751	0.745686
82	1	0	-5.268820	0.229352	1.073589
83	1	0	-5.992350	-4.672548	0.848933
84	6	0	-6.904304	-2.727261	0.677936
85	1	0	-7.526798	-0.666320	0.581859
86	1	0	-7.892728	-3.120525	0.458806

Pt-2 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.523820	1.611245	-1.981054
2	6	0	1.664683	2.301899	-2.030737
3	6	0	-0.665708	2.256644	-2.111412
4	78	0	0.297418	-0.487540	-1.668079
5	1	0	2.570152	1.716816	-1.903791
6	6	0	1.689368	3.677188	-2.222529
7	6	0	-0.708443	3.631995	-2.306051
8	6	0	-1.872643	1.407424	-2.030880
9	7	0	-1.612097	0.101286	-1.863095
10	6	0	-0.572978	-2.261785	-1.422908
11	6	0	2.155510	-1.033939	-1.442287
12	1	0	2.638162	4.201226	-2.251190
13	6	0	0.481301	4.349829	-2.360603
14	1	0	-1.659441	4.142066	-2.398926
15	6	0	-3.193775	1.837931	-2.096772
16	6	0	-2.561197	-0.846966	-1.733806
17	6	0	-1.998930	-2.181729	-1.495426
18	6	0	-0.012633	-3.514008	-1.156765
19	6	0	3.337302	-1.294180	-1.219893
20	1	0	0.459320	5.425282	-2.502167
21	1	0	-3.437413	2.886471	-2.218975
22	6	0	-4.204220	0.882601	-1.990674
23	6	0	-3.900094	-0.462408	-1.812054
24	6	0	-2.794266	-3.314696	-1.308284
25	1	0	1.067702	-3.601863	-1.082259
26	6	0	-0.813822	-4.641641	-0.966087
27	6	0	4.682442	-1.588740	-0.862337
28	1	0	-5.242675	1.195406	-2.033568
29	1	0	-4.692062	-1.194112	-1.704657
30	6	0	-2.202973	-4.546213	-1.041667
31	1	0	-3.877249	-3.238325	-1.352443
32	1	0	-0.349579	-5.602011	-0.753453
33	6	0	5.059017	-2.890082	-0.477770
34	6	0	5.661191	-0.576817	-0.835627
35	1	0	-2.823835	-5.424678	-0.890620
36	1	0	4.311835	-3.678442	-0.492455
37	6	0	6.360076	-3.162630	-0.071862

38	6	0	6.960814	-0.855485	-0.428013
39	1	0	5.382006	0.431151	-1.129111
40	1	0	6.629159	-4.172656	0.225684
41	6	0	7.316509	-2.147583	-0.041507
42	1	0	7.700190	-0.059182	-0.409966
43	1	0	8.331977	-2.362392	0.279029
44	1	0	1.217150	5.361537	0.878596
45	6	0	0.319033	4.752708	0.945609
46	6	0	0.413491	3.378379	1.179825
47	6	0	-0.926756	5.349654	0.784715
48	6	0	1.697574	2.682674	1.330287
49	6	0	-0.758508	2.563415	1.268585
50	6	0	-2.079135	4.567093	0.854558
51	1	0	-0.997187	6.417323	0.598227
52	7	0	1.550367	1.361880	1.562985
53	6	0	2.990975	3.201240	1.246203
54	6	0	-1.993766	3.195124	1.095711
55	78	0	-0.327161	0.649988	1.605509
56	1	0	-3.054202	5.030171	0.721097
57	6	0	2.574939	0.508866	1.728002
58	6	0	4.073678	2.343276	1.411207
59	1	0	3.150321	4.255394	1.049994
60	1	0	-2.899847	2.597812	1.143839
61	7	0	0.822336	-1.121377	1.953708
62	6	0	-2.151323	-0.037430	1.629728
63	6	0	2.161403	-0.890627	1.956625
64	6	0	3.880180	0.984953	1.659625
65	1	0	5.083881	2.734429	1.342912
66	6	0	0.362840	-2.364640	2.102840
67	6	0	-3.280858	-0.520390	1.569347
68	6	0	3.062610	-1.931185	2.147865
69	1	0	4.727933	0.321210	1.774877
70	1	0	-0.716100	-2.472597	2.064611
71	6	0	1.210849	-3.450715	2.283318
72	6	0	-4.578583	-1.076537	1.392441
73	6	0	2.581843	-3.226046	2.311623
74	1	0	4.128947	-1.741191	2.145686
75	1	0	0.795255	-4.446218	2.391732
76	6	0	-5.693965	-0.247955	1.165080
77	6	0	-4.771937	-2.470523	1.387078
78	1	0	3.276403	-4.048594	2.448863
79	1	0	-5.555400	0.829490	1.161970
80	6	0	-6.949569	-0.794963	0.930011

81	6	0	-6.030280	-3.012342	1.149768
82	1	0	-3.917414	-3.119673	1.552827
83	1	0	-7.796824	-0.138169	0.751168
84	6	0	-7.124430	-2.179175	0.917903
85	1	0	-6.157075	-4.091763	1.142822
86	1	0	-8.106145	-2.604876	0.730269

Rh(terpy)Br dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.003444	-0.614334	1.454267
2	7	0	-2.012348	-0.946621	1.369767
3	7	0	-0.005800	-2.397036	0.740674
4	7	0	2.004561	-0.952926	1.372319
5	35	0	-0.000119	1.573006	2.692410
6	6	0	-2.999239	-0.119477	1.744091
7	6	0	-2.337541	-2.165600	0.844039
8	6	0	-1.189528	-3.000899	0.485500
9	6	0	1.176379	-3.004558	0.486957
10	6	0	2.326566	-2.172906	0.847039
11	6	0	2.993531	-0.128983	1.748168
12	1	0	-2.671603	0.832021	2.149241
13	6	0	-4.339674	-0.454667	1.626461
14	6	0	-3.665962	-2.554716	0.693847
15	6	0	-1.214643	-4.283726	-0.050507
16	6	0	1.198173	-4.287448	-0.049023
17	6	0	3.653958	-2.566275	0.698735
18	6	0	4.333045	-0.468456	1.632490
19	1	0	2.668311	0.823493	2.152967
20	1	0	-5.098083	0.252440	1.943613
21	6	0	-4.680479	-1.694074	1.091088
22	1	0	-3.902428	-3.524737	0.270939
23	1	0	-2.157175	-4.777720	-0.258052
24	6	0	-0.009059	-4.926212	-0.320489
25	1	0	2.139416	-4.784368	-0.255408
26	1	0	3.887946	-3.536976	0.276010
27	6	0	4.670643	-1.708916	1.097530
28	1	0	5.093248	0.236228	1.950735
29	1	0	-5.719865	-1.985233	0.980045
30	1	0	-0.010341	-5.926487	-0.740053
31	1	0	5.709255	-2.003369	0.987942
32	45	0	0.003003	0.614314	-1.454225
33	7	0	2.012142	0.945204	-1.370557
34	7	0	0.006888	2.397007	-0.740627
35	7	0	-2.004784	0.954313	-1.371456
36	35	0	-0.002114	-1.573005	-2.692390
37	6	0	2.998278	0.117393	-1.745415

38	6	0	2.338431	2.163880	-0.844810
39	6	0	1.191152	2.999998	-0.485831
40	6	0	-1.174751	3.005426	-0.486576
41	6	0	-2.325678	2.174598	-0.846188
42	6	0	-2.994502	0.131114	-1.746954
43	1	0	2.669767	-0.833633	-2.150996
44	6	0	4.339007	0.451528	-1.628158
45	6	0	3.667199	2.551983	-0.695057
46	6	0	1.217386	4.282813	0.050158
47	6	0	-1.195424	4.288370	0.049305
48	6	0	-3.652720	2.569015	-0.697534
49	6	0	-4.333725	0.471662	-1.630952
50	1	0	-2.670152	-0.821652	-2.151770
51	1	0	5.096763	-0.256123	-1.945669
52	6	0	4.680928	1.690588	-1.092678
53	1	0	3.904543	3.521792	-0.272159
54	1	0	2.160354	4.776090	0.257432
55	6	0	0.012363	4.926229	0.320425
56	1	0	-2.136232	4.786019	0.255913
57	1	0	-3.885832	3.539982	-0.274933
58	6	0	-4.670192	1.712430	-1.095986
59	1	0	-5.094577	-0.232388	-1.949048
60	1	0	5.720571	1.980941	-0.981939
61	1	0	0.014515	5.926526	0.739934
62	1	0	-5.708539	2.007748	-0.986209

Rh(terpy)CCCH$_3$ dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.000118	0.485480	-1.501327
2	7	0	-2.003582	0.848103	-1.442943
3	7	0	-0.000464	2.347481	-0.888304
4	7	0	2.003195	0.848858	-1.443021
5	6	0	0.000175	-1.337220	-2.304089
6	6	0	-2.994054	0.001610	-1.764829
7	6	0	-2.327864	2.097917	-0.987464
8	6	0	-1.182513	2.960058	-0.673798
9	6	0	1.181364	2.960490	-0.673796
10	6	0	2.327023	2.098758	-0.987449
11	6	0	2.993986	0.002707	-1.764825
12	6	0	0.000302	-2.465831	-2.802387
13	1	0	-2.666410	-0.972666	-2.110687
14	6	0	-4.333861	0.343731	-1.665833
15	6	0	-3.656867	2.494518	-0.860964
16	6	0	-1.209804	4.274657	-0.218386
17	6	0	1.208179	4.275097	-0.218383
18	6	0	3.655881	2.495799	-0.860813
19	6	0	4.333672	0.345265	-1.665679
20	1	0	2.666716	-0.971680	-2.110718
21	6	0	0.000537	-3.815657	-3.362794
22	1	0	-5.093372	-0.380542	-1.938956
23	6	0	-4.673255	1.613817	-1.205645
24	1	0	-3.891778	3.488163	-0.495438
25	1	0	-2.150071	4.785024	-0.041367
26	6	0	-0.000934	4.928905	0.009767
27	1	0	2.148257	4.785813	-0.041372
28	1	0	3.890429	3.489501	-0.495215
29	6	0	4.672598	1.615448	-1.205418
30	1	0	5.093451	-0.378752	-1.938735
31	1	0	0.000384	-3.805804	-4.461146
32	1	0	0.881640	-4.388734	-3.045069
33	1	0	-0.880217	-4.389142	-3.044834
34	1	0	-5.712242	1.912517	-1.111528
35	1	0	-0.001118	5.952982	0.367977
36	1	0	5.711477	1.914486	-1.111177
37	1	0	-0.881357	4.388788	3.045086

38	6	0	0.000016	3.815865	3.362349
39	6	0	0.000093	2.465938	2.802167
40	1	0	0.000829	3.806158	4.460696
41	1	0	0.880509	4.389401	3.043771
42	6	0	0.000135	1.337303	2.303921
43	45	0	0.000214	-0.485459	1.501266
44	7	0	2.003627	-0.848348	1.442862
45	7	0	0.000302	-2.347447	0.888196
46	7	0	-2.003143	-0.848620	1.443124
47	6	0	2.994223	-0.002059	1.764888
48	6	0	2.327734	-2.098180	0.987313
49	6	0	1.182267	-2.960114	0.673492
50	6	0	-1.181609	-2.960266	0.673627
51	6	0	-2.327146	-2.098491	0.987610
52	6	0	-2.993804	-0.002484	1.765351
53	1	0	2.666741	0.972269	2.110748
54	6	0	4.333980	-0.344422	1.666018
55	6	0	3.656675	-2.495032	0.860958
56	6	0	1.209377	-4.274587	0.217704
57	6	0	-1.208608	-4.274742	0.217847
58	6	0	-3.656052	-2.495534	0.861483
59	6	0	-4.333530	-0.345045	1.666724
60	1	0	-2.666400	0.971889	2.111159
61	1	0	5.093589	0.379703	1.939261
62	6	0	4.673193	-1.614546	1.205807
63	1	0	3.891430	-3.488713	0.495431
64	1	0	2.149569	-4.785009	0.040452
65	6	0	0.000413	-4.928622	-0.010563
66	1	0	-2.148756	-4.785285	0.040706
67	1	0	-3.890733	-3.489243	0.495990
68	6	0	-4.672636	-1.615207	1.206542
69	1	0	-5.093198	0.378957	1.940127
70	1	0	5.712135	-1.913445	1.111817
71	1	0	0.000457	-5.952579	-0.369113
72	1	0	-5.711550	-1.914259	1.112737

Rh(terpy)CN dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.002425	0.714311	-1.339353
2	7	0	-2.008582	1.069594	-1.235542
3	7	0	-0.004558	2.428847	-0.382656
4	7	0	2.002814	1.075230	-1.236546
5	6	0	-0.000631	-0.868621	-2.523995
6	6	0	-2.998913	0.312972	-1.731724
7	6	0	-2.332572	2.204621	-0.543105
8	6	0	-1.187177	2.984631	-0.057340
9	6	0	1.176656	2.988038	-0.058074
10	6	0	2.323985	2.211222	-0.544416
11	6	0	2.994995	0.321273	-1.733084
12	7	0	0.000282	-1.769628	-3.280637
13	1	0	-2.680470	-0.576096	-2.263480
14	6	0	-4.338659	0.638245	-1.580279
15	6	0	-3.659676	2.576729	-0.350699
16	6	0	-1.216299	4.185008	0.645664
17	6	0	1.202760	4.188488	0.644914
18	6	0	3.650146	2.587050	-0.352715
19	6	0	4.333912	0.650235	-1.582281
20	1	0	2.678761	-0.568727	-2.264597
21	1	0	-5.097580	-0.010110	-2.003697
22	6	0	-4.676746	1.789964	-0.875566
23	1	0	-3.893952	3.477498	0.205620
24	1	0	-2.156414	4.651425	0.917273
25	6	0	-0.007517	4.781074	0.998150
26	1	0	2.141695	4.657578	0.915999
27	1	0	3.882187	3.488561	0.203339
28	6	0	4.669137	1.803003	-0.877912
29	1	0	5.094432	0.003900	-2.005916
30	1	0	-5.715093	2.070517	-0.732894
31	1	0	-0.008691	5.716397	1.547830
32	1	0	5.706773	2.086432	-0.735743
33	45	0	0.002516	-0.714321	1.339372
34	7	0	2.008636	-1.069783	1.235468
35	7	0	0.004451	-2.428839	0.382644
36	7	0	-2.002760	-1.075059	1.236649
37	6	0	0.000901	0.868607	2.524020

38	6	0	2.999056	-0.313247	1.731603
39	6	0	2.332493	-2.204834	0.543010
40	6	0	1.187007	-2.984731	0.057280
41	6	0	-1.176827	-2.987912	0.058092
42	6	0	-2.324065	-2.210992	0.544484
43	6	0	-2.994851	-0.321029	1.733256
44	7	0	0.000142	1.769572	3.280712
45	1	0	2.680717	0.575848	2.263375
46	6	0	4.338767	-0.638639	1.580093
47	6	0	3.659555	-2.577054	0.350531
48	6	0	1.215991	-4.185105	-0.645735
49	6	0	-1.203070	-4.188349	-0.644914
50	6	0	-3.650269	-2.586682	0.352813
51	6	0	-4.333805	-0.649851	1.582482
52	1	0	-2.678512	0.568915	2.264800
53	1	0	5.097766	0.009645	2.003479
54	6	0	4.676718	-1.790382	0.875356
55	1	0	3.893725	-3.477831	-0.205820
56	1	0	2.156052	-4.651609	-0.917381
57	6	0	0.007140	-4.781047	-0.998196
58	1	0	-2.142058	-4.657346	-0.915975
59	1	0	-3.882417	-3.488157	-0.203254
60	6	0	-4.669167	-1.802555	0.878074
61	1	0	-5.094246	-0.003456	2.006167
62	1	0	5.715034	-2.071019	0.732621
63	1	0	0.008206	-5.716363	-1.547888
64	1	0	-5.706836	-2.085882	0.735938

Rh(terpy)CO dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.000755	-0.615103	1.372678
2	7	0	-2.018113	-0.995296	1.273114
3	7	0	0.001031	-2.382801	0.455086
4	7	0	2.019820	-0.994081	1.272130
5	6	0	0.000640	0.895276	2.441238
6	6	0	-3.012139	-0.247539	1.770001
7	6	0	-2.330554	-2.149872	0.613166
8	6	0	-1.180916	-2.924756	0.121367
9	6	0	1.183151	-2.924081	0.120872
10	6	0	2.332591	-2.148623	0.612256
11	6	0	3.013679	-0.245780	1.768526
12	8	0	0.000841	1.815940	3.136944
13	1	0	-2.718966	0.656414	2.289298
14	6	0	-4.349575	-0.597321	1.638485
15	6	0	-3.650058	-2.550257	0.445708
16	6	0	-1.210109	-4.102922	-0.618568
17	6	0	1.212715	-4.102196	-0.619135
18	6	0	3.652227	-2.548498	0.444538
19	6	0	4.351223	-0.595012	1.636682
20	1	0	2.720253	0.658200	2.287672
21	1	0	-5.112241	0.046905	2.060306
22	6	0	-4.675158	-1.766867	0.963690
23	1	0	-3.875438	-3.469388	-0.082540
24	1	0	-2.147916	-4.560414	-0.909578
25	6	0	0.001392	-4.682697	-0.988313
26	1	0	2.150677	-4.559063	-0.910627
27	1	0	3.877819	-3.467724	-0.083464
28	6	0	4.677140	-1.764601	0.962142
29	1	0	5.113711	0.049599	2.058237
30	1	0	-5.709575	-2.068601	0.839994
31	1	0	0.001528	-5.597883	-1.570369
32	1	0	5.711657	-2.065984	0.838441
33	1	0	2.719282	-0.655814	-2.289103
34	6	0	3.012295	0.248033	-1.769495
35	7	0	2.018139	0.995683	-1.272762
36	6	0	4.349677	0.598007	-1.637844
37	45	0	-0.000576	0.615226	-1.372804

38	6	0	2.330348	2.150220	-0.612659
39	1	0	5.112472	-0.046021	-2.059734
40	6	0	4.675049	1.767461	-0.962790
41	7	0	-0.001282	2.382845	-0.455063
42	7	0	-2.019662	0.993834	-1.272681
43	6	0	0.000053	-0.895331	-2.441141
44	6	0	3.649789	2.550674	-0.444859
45	6	0	1.180505	2.924962	-0.121081
46	1	0	5.709422	2.069260	-0.838893
47	6	0	-1.183566	2.923841	-0.120970
48	6	0	-2.332757	2.148222	-0.612682
49	6	0	-3.013295	0.245450	-1.769403
50	8	0	0.000506	-1.816159	-3.136621
51	1	0	3.874955	3.469700	0.083667
52	6	0	1.209369	4.103074	0.618961
53	6	0	-1.213469	4.101804	0.619260
54	6	0	-3.652484	2.547832	-0.445139
55	6	0	-4.350929	0.594460	-1.637815
56	1	0	-2.719638	-0.658472	-2.288518
57	1	0	2.147050	4.560754	0.910085
58	6	0	-0.002306	4.682520	0.988645
59	1	0	-2.151541	4.558425	0.910789
60	1	0	-3.878363	3.466815	0.083151
61	6	0	-4.677162	1.763834	-0.963051
62	1	0	-5.113237	-0.050253	-2.059541
63	1	0	-0.002722	5.597618	1.570840
64	1	0	-5.711752	2.064958	-0.839317

Rh(terpy)I dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.001662	-0.083891	1.609169
2	7	0	-2.014076	-0.435112	1.630403
3	7	0	0.002907	-2.006300	1.518659
4	7	0	2.017897	-0.432379	1.628135
5	53	0	0.000256	2.580549	2.255933
6	6	0	-3.013155	0.457654	1.691713
7	6	0	-2.330181	-1.762191	1.546461
8	6	0	-1.178370	-2.664167	1.494772
9	6	0	1.185044	-2.662560	1.493290
10	6	0	2.335687	-1.759021	1.543584
11	6	0	3.015867	0.461711	1.688278
12	1	0	-2.705557	1.495437	1.750816
13	6	0	-4.350623	0.089763	1.686519
14	6	0	-3.653811	-2.192819	1.528685
15	6	0	-1.201525	-4.053637	1.443179
16	6	0	1.210031	-4.052005	1.441666
17	6	0	3.659868	-2.187862	1.523969
18	6	0	4.353822	0.095616	1.681251
19	1	0	2.706976	1.499079	1.747921
20	1	0	-5.115177	0.856902	1.738095
21	6	0	-4.679232	-1.259875	1.604178
22	1	0	-3.877766	-3.251170	1.457666
23	1	0	-2.143293	-4.590312	1.426334
24	6	0	0.004708	-4.748214	1.414296
25	1	0	2.152506	-4.587402	1.423669
26	1	0	3.885151	-3.245895	1.452433
27	6	0	4.684138	-1.253560	1.598240
28	1	0	5.117413	0.863776	1.731921
29	1	0	-5.715342	-1.581787	1.592379
30	1	0	0.005416	-5.832131	1.374479
31	1	0	5.720664	-1.574075	1.584972
32	45	0	-0.001645	0.083893	-1.609179
33	7	0	2.014074	0.435297	-1.630339
34	7	0	-0.003063	2.006301	-1.518679
35	7	0	-2.017899	0.432191	-1.628176
36	53	0	0.000012	-2.580543	-2.255965
37	6	0	3.013242	-0.457379	-1.691523

38	6	0	2.330047	1.762407	-1.546411
39	6	0	1.178150	2.664277	-1.494788
40	6	0	-1.185264	2.662452	-1.493353
41	6	0	-2.335820	1.758803	-1.543627
42	6	0	-3.015780	-0.461998	-1.688341
43	1	0	2.705746	-1.495193	-1.750617
44	6	0	4.350675	-0.089362	-1.686217
45	6	0	3.653635	2.193160	-1.528539
46	6	0	1.201177	4.053753	-1.443251
47	6	0	-1.210380	4.051896	-1.441789
48	6	0	-3.660044	2.187510	-1.524009
49	6	0	-4.353770	-0.096037	-1.681321
50	1	0	-2.706784	-1.499334	-1.748000
51	1	0	5.115306	-0.856431	-1.737687
52	6	0	4.679148	1.260310	-1.603903
53	1	0	3.877485	3.251534	-1.457518
54	1	0	2.142895	4.590515	-1.426416
55	6	0	-0.005121	4.748219	-1.414425
56	1	0	-2.152904	4.587208	-1.423835
57	1	0	-3.885432	3.245521	-1.452478
58	6	0	-4.684221	1.253106	-1.598293
59	1	0	-5.117283	-0.864272	-1.732012
60	1	0	5.715228	1.582319	-1.592010
61	1	0	-0.005932	5.832137	-1.374659
62	1	0	-5.720779	1.573518	-1.585033

Rh(terpy)CNCH$_3$ dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.000089	0.284753	1.477515
2	7	0	2.013047	0.665771	1.472530
3	7	0	-0.000087	2.203154	1.007224
4	7	0	-2.013216	0.665708	1.472460
5	6	0	-0.000102	-1.508608	2.155972
6	6	0	3.006493	-0.182800	1.770460
7	6	0	2.330299	1.942589	1.101804
8	6	0	1.181877	2.813659	0.813991
9	6	0	-1.182063	2.813623	0.813951
10	6	0	-2.330476	1.942522	1.101708
11	6	0	-3.006664	-0.182875	1.770347
12	7	0	-0.000097	-2.592277	2.602459
13	1	0	2.704922	-1.183504	2.055741
14	6	0	4.344737	0.182437	1.721868
15	6	0	3.652381	2.365872	1.029297
16	6	0	1.210744	4.139558	0.391143
17	6	0	-1.210951	4.139531	0.391124
18	6	0	-3.652563	2.365773	1.029118
19	6	0	-4.344913	0.182337	1.721680
20	1	0	-2.705093	-1.183570	2.055658
21	6	0	-0.000118	-3.873117	3.196585
22	1	0	5.106405	-0.546603	1.973608
23	6	0	4.674808	1.478770	1.343666
24	1	0	3.880650	3.383125	0.732758
25	1	0	2.149085	4.655536	0.224899
26	6	0	-0.000109	4.795833	0.180484
27	1	0	-2.149301	4.655495	0.224879
28	1	0	-3.880838	3.383016	0.732548
29	6	0	-4.674991	1.478656	1.343442
30	1	0	-5.106578	-0.546717	1.973388
31	1	0	-0.000220	-3.774070	4.285375
32	1	0	-0.890459	-4.424001	2.883231
33	1	0	0.890310	-4.423956	2.883401
34	1	0	5.710522	1.796919	1.291676
35	1	0	-0.000118	5.828510	-0.151686
36	1	0	-5.710709	1.796782	1.291385
37	45	0	0.000080	-0.284736	-1.477454

38	7	0	-2.013048	-0.665755	-1.472509
39	7	0	0.000082	-2.203147	-1.007223
40	7	0	2.013214	-0.665690	-1.472393
41	6	0	0.000068	1.508604	-2.155968
42	6	0	-3.006494	0.182832	-1.770398
43	6	0	-2.330304	-1.942586	-1.101825
44	6	0	-1.181885	-2.813669	-0.814049
45	6	0	1.182056	-2.813629	-0.813974
46	6	0	2.330470	-1.942522	-1.101696
47	6	0	3.006664	0.182907	-1.770229
48	7	0	0.000084	2.592253	-2.602504
49	1	0	-2.704923	1.183543	-2.055654
50	6	0	-4.344739	-0.182399	-1.721801
51	6	0	-3.652389	-2.365859	-1.029308
52	6	0	-1.210755	-4.139597	-0.391291
53	6	0	1.210939	-4.139554	-0.391201
54	6	0	3.652557	-2.365779	-1.029126
55	6	0	4.344912	-0.182308	-1.721575
56	1	0	2.705093	1.183618	-2.055486
57	6	0	0.000255	3.872981	-3.196867
58	1	0	-5.106406	0.546654	-1.973507
59	6	0	-4.674814	-1.478742	-1.343634
60	1	0	-3.880662	-3.383117	-0.732785
61	1	0	-2.149099	-4.655596	-0.225124
62	6	0	0.000097	-4.795873	-0.180624
63	1	0	2.149288	-4.655518	-0.224951
64	1	0	3.880831	-3.383035	-0.732601
65	6	0	4.674987	-1.478648	-1.343403
66	1	0	5.106579	0.546758	-1.973244
67	1	0	0.891140	4.423471	-2.884369
68	1	0	-0.000613	3.773734	-4.285639
69	1	0	-0.889633	4.424328	-2.883045
70	1	0	-5.710530	-1.796882	-1.291629
71	1	0	0.000104	-5.828567	0.151490
72	1	0	5.710704	-1.796777	-1.291357

Rh(terpy)NH_3 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.008917	-0.762551	1.334710
2	7	0	-2.024914	-1.111535	1.204735
3	7	0	0.005190	-2.394951	0.313905
4	7	0	2.007209	-1.090656	1.240970
5	7	0	0.012820	0.919303	2.650216
6	6	0	-3.034259	-0.407662	1.735326
7	6	0	-2.330516	-2.208762	0.447997
8	6	0	-1.171572	-2.935635	-0.076134
9	6	0	1.195764	-2.928700	-0.046737
10	6	0	2.338129	-2.190084	0.498168
11	6	0	2.998373	-0.365471	1.778607
12	1	0	0.516387	1.725569	2.282801
13	1	0	0.473591	0.668230	3.524377
14	1	0	-0.902485	1.273071	2.921998
15	1	0	-2.758930	0.456861	2.326555
16	6	0	-4.368192	-0.742978	1.556510
17	6	0	-3.648724	-2.594528	0.225206
18	6	0	-1.182365	-4.065020	-0.889707
19	6	0	1.232554	-4.056261	-0.862569
20	6	0	3.664554	-2.559816	0.298630
21	6	0	4.339081	-0.682767	1.618855
22	1	0	2.699362	0.499578	2.358436
23	1	0	-5.138499	-0.132005	2.013064
24	6	0	-4.683273	-1.856934	0.785102
25	1	0	-3.863071	-3.468094	-0.379869
26	1	0	-2.117881	-4.504082	-1.216113
27	6	0	0.031192	-4.620926	-1.286981
28	1	0	2.178233	-4.488462	-1.168260
29	1	0	3.900144	-3.435956	-0.294742
30	6	0	4.680304	-1.800840	0.864399
31	1	0	5.094755	-0.055641	2.078011
32	1	0	-5.715508	-2.146617	0.620033
33	1	0	0.041840	-5.496628	-1.926487
34	1	0	5.718798	-2.076913	0.716158
35	1	0	0.516774	-1.725230	-2.282458
36	7	0	0.012489	-0.919478	-2.650003
37	45	0	-0.009709	0.762582	-1.334766

38	1	0	0.472785	-0.668346	-3.524394
39	1	0	-0.902651	-1.274012	-2.921338
40	7	0	2.006336	1.091493	-1.241253
41	7	0	0.003886	2.394980	-0.313962
42	7	0	-2.025818	1.110759	-1.204567
43	6	0	2.997756	0.366672	-1.778908
44	6	0	2.336882	2.191040	-0.498465
45	6	0	1.194278	2.929190	0.046570
46	6	0	-1.173052	2.935107	0.076329
47	6	0	-2.331769	2.207830	-0.447743
48	6	0	-3.034934	0.406587	-1.735192
49	1	0	2.699077	-0.498490	-2.358741
50	6	0	4.338355	0.684448	-1.619184
51	6	0	3.663178	2.561256	-0.298957
52	6	0	1.230709	4.056685	0.862514
53	6	0	-1.184207	4.064349	0.890090
54	6	0	-3.650101	2.593143	-0.224907
55	6	0	-4.368976	0.741444	-1.556322
56	1	0	-2.759330	-0.457799	-2.326490
57	1	0	5.094241	0.057585	-2.078348
58	6	0	4.679193	1.802648	-0.864743
59	1	0	3.898466	3.437466	0.294429
60	1	0	2.176247	4.489278	1.168083
61	6	0	0.029172	4.620751	1.287219
62	1	0	-2.119860	4.502921	1.216758
63	1	0	-3.864730	3.466626	0.380188
64	6	0	-4.684415	1.855237	-0.784829
65	1	0	-5.139086	0.130249	-2.012912
66	1	0	5.717590	2.079091	-0.716511
67	1	0	0.039541	5.496370	1.926845
68	1	0	-5.716744	2.144575	-0.619738

Rh(terpy)PH_3 dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.004019	0.652950	1.362924
2	7	0	2.022783	1.021936	1.247547
3	7	0	-0.003751	2.382292	0.426588
4	7	0	-2.017540	1.009691	1.260180
5	15	0	0.009633	-1.026418	2.896559
6	6	0	3.032831	0.279804	1.722932
7	6	0	2.328786	2.173957	0.577192
8	6	0	1.174794	2.943735	0.098969
9	6	0	-1.187654	2.939218	0.111006
10	6	0	-2.334101	2.162733	0.596292
11	6	0	-3.020999	0.258901	1.736481
12	1	0	-0.050827	-2.405349	2.581679
13	1	0	1.101647	-1.101733	3.790380
14	1	0	-1.022173	-1.025095	3.862013
15	1	0	2.758347	-0.631018	2.239685
16	6	0	4.366669	0.633154	1.576216
17	6	0	3.645948	2.579456	0.391859
18	6	0	1.196884	4.141154	-0.610957
19	6	0	-1.221471	4.137011	-0.597769
20	6	0	-3.654551	2.561584	0.420192
21	6	0	-4.357638	0.604755	1.597692
22	1	0	-2.739424	-0.653462	2.247156
23	1	0	5.136168	-0.011282	1.985448
24	6	0	4.681455	1.805243	0.899081
25	1	0	3.859767	3.497313	-0.143527
26	1	0	2.133599	4.608218	-0.890735
27	6	0	-0.015250	4.731249	-0.961859
28	1	0	-2.162768	4.600779	-0.867385
29	1	0	-3.876616	3.480533	-0.109963
30	6	0	-4.682816	1.778719	0.928747
31	1	0	-5.121212	-0.046654	2.006970
32	1	0	5.713035	2.111633	0.763160
33	1	0	-0.019883	5.661662	-1.519120
34	1	0	-5.716899	2.079562	0.799663
35	1	0	-0.049552	2.405399	-2.581605
36	15	0	0.009767	1.026429	-2.896530
37	45	0	0.003686	-0.652953	-1.362920

38	1	0	-1.022406	1.025886	-3.861592
39	1	0	1.101512	1.100966	-3.790748
40	7	0	-2.017955	-1.009272	-1.260194
41	7	0	-0.004459	-2.382291	-0.426583
42	7	0	2.022358	-1.022367	-1.247551
43	6	0	-3.021254	-0.258293	-1.736531
44	6	0	-2.334762	-2.162230	-0.596273
45	6	0	-1.188480	-2.938954	-0.110984
46	6	0	1.173968	-2.943985	-0.098964
47	6	0	2.328121	-2.174462	-0.577215
48	6	0	3.032556	-0.280440	-1.722941
49	1	0	-2.739486	0.653977	-2.247261
50	6	0	-4.357967	-0.603857	-1.597726
51	6	0	-3.655297	-2.560792	-0.420153
52	6	0	-1.222552	-4.136730	0.597807
53	6	0	1.195803	-4.141394	0.610988
54	6	0	3.645199	-2.580252	-0.391923
55	6	0	4.366320	-0.634084	-1.576261
56	1	0	2.758252	0.630457	-2.239662
57	1	0	-5.121400	0.047698	-2.007033
58	6	0	-4.683396	-1.777722	-0.928730
59	1	0	-3.877559	-3.479674	0.110035
60	1	0	-2.163949	-4.600291	0.867429
61	6	0	-0.016454	-4.731220	0.961905
62	1	0	2.132418	-4.608654	0.890778
63	1	0	3.858827	-3.498166	0.143440
64	6	0	4.680864	-1.806258	-0.899159
65	1	0	5.135953	0.010191	-1.985494
66	1	0	-5.717544	-2.078333	-0.799627
67	1	0	-0.021284	-5.661622	1.519184
68	1	0	5.712379	-2.112882	-0.763273

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