Supporting Information

Phospha- and Arsa-Bridged Cyclononatetraenides: Novel Zwitterionic 10π Aromatic Hemispheres

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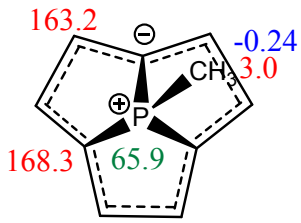
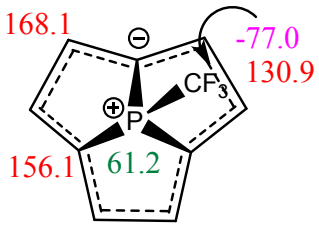
Contents

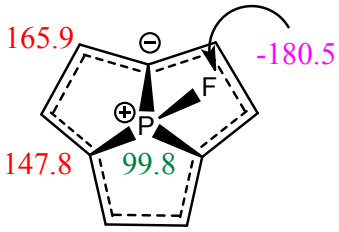
B3LYP/6-311++G(d,p) ^{13}C NMR ^{1}H NMR ^{31}P NMR ^{19}F NMR



NICS(1) = -6.19
NICS(1)$_{zz}$= -15.24



NICS(1) = -5.50
NICS(1)$_{zz}$= -15.34



NICS(1) = -4.62
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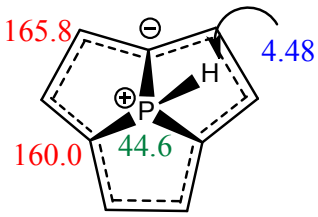
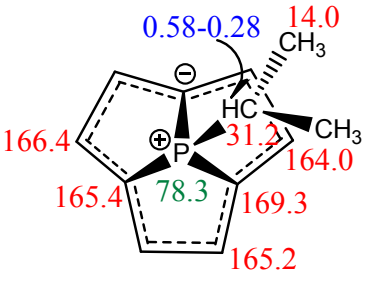
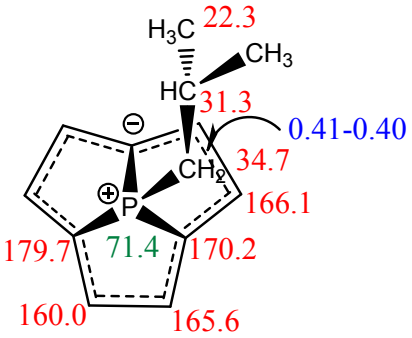


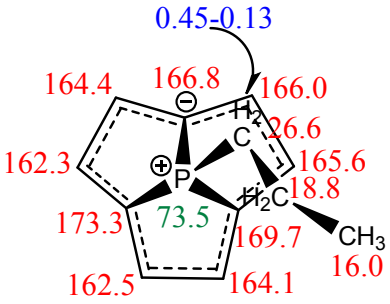
NICS(1) = -5.19
NICS(1)$_{zz}$= -13.25



NICS(1) = -5.68
NICS(1)$_{zz}$= -15.45

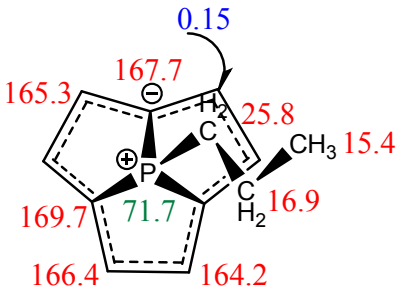


NICS(1) = -5.52
NICS(1)$_{zz}$= -12.82



NICS(1) = -5.23
NICS(1)$_{zz}$= -12.40

same compound, different rotamers



NICS(1) = -5.96
NICS(1)$_{zz}$= -14.52

Figure S1. GIAO NMR and NICS data for the phosphatriquinane-derived zwitterions with different R groups at phosphorus.

B3LYP/6-311++G(d,p) ^{13}C NMR ^{1}H NMR ^{31}P NMR ^{19}F NMR

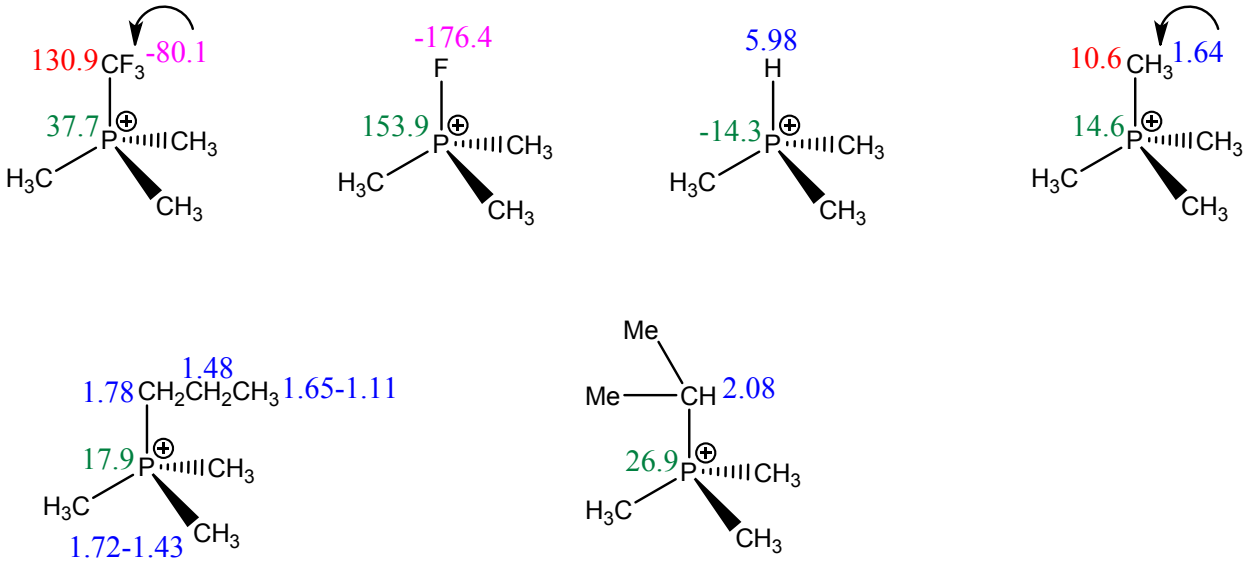
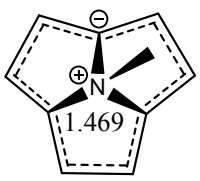


Figure S2. Multinuclear GIAO NMR data for model systems**.**



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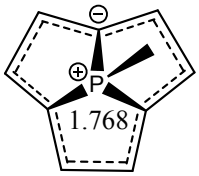
Natural bond order N-C (bridge) = 0.96
Wiberg bond order N-C (bridge) = 0.85



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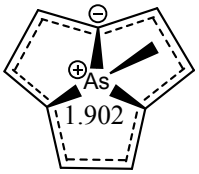
P-C (bridge) = 0.95
P-C (bridge) = 0.92



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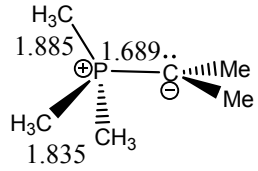
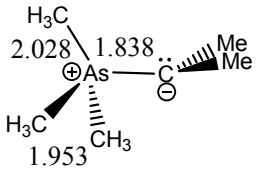
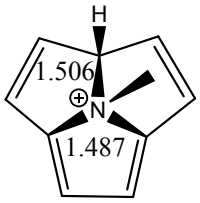
As-C (bridge) = 0.94
As-C (bridge) = 0.90



Natural bond order P-C_{sp2} = 0.97
Wiberg bond order P-C_{sp2} = 1.29



As-C_{sp2} = 0.94
As-C_{sp2} = 1.23



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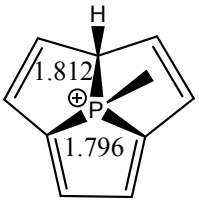

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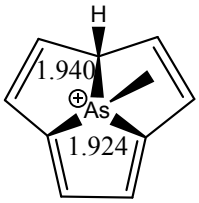

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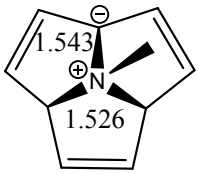
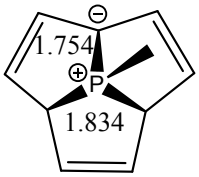


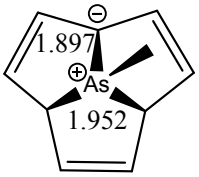
S1

Natural bond order N-C (anionic) = 0.96
Wiberg bond order N-C (anionic) = 0.80



S2

P-C (anionic) = 0.96
P-C (anionic) = 1.03

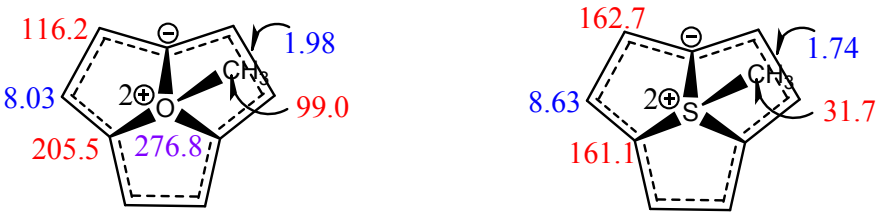


S3

As-C (anionic) = 0.95
As-C (anionic) = 0.97

Figure S3. Selected bond-lengths and computed natural bond orders (NBO) and Wiberg bond orders in the zwitterions and comparison with simple ylides.

B3LYP/6-311++G(d,p) ^{1}H NMR ^{13}C NMR ^{17}O NMR



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NICS(1) = -12.48

NICS(1)$_{zz}$= -29.77

22

NICS(1) = -7.48

NICS(1)$_{zz}$= -15.92

Figure S4. Multinuclear NMR and NICS data for the oxatriquinane and thiatriquinane derivatives.

Table S1. Solvation effect on NICS values for P-R structures in Figure 3 (ppm).

R	NICS(1)				NICS(1)$_{zz}$			
	Gas Phase	*n*-pentane	CH_2Cl_2	CH_3CN	Gas Phase	*n*-pentane	CH_2Cl_2	CH_3CN
CH_3	-6.19	-5.96	-5.84	-5.91	-15.24	-15.10	-14.88	-14.93
CF_3	-5.50	-5.47	-5.35	-5.33	-15.34	-15.26	-14.97	-14.86
F	-4.62	-4.55	-4.43	-4.39	-14.55	-14.38	-14.07	-13.97
H	-5.19	-5.15	-5.08	-5.06	-13.25	-13.12	-12.87	-12.81
iso-Pr	-5.68	-5.53	-5.47	-5.45	-15.45	-15.97	-15.79	-15.75
sec-Bu	-5.52	-5.46	-5.39	-5.38	-12.82	-12.55	-12.70	-12.52
n-Pr	-5.96	-5.87	-5.77	-5.76	-14.52	-14.38	-14.18	-14.14

Table S2. Solvation effect on selected chemical shifts for P-R structures shown in Figure 3 (ppm).

R	Chemical shift			
	Gas Phase	*n*-pentane	CH_2Cl_2	CH_3CN
CH_3	-0.24	-0.16	-0.04	-0.06
CF_3	-77.0	-77.6	-78.07	-78.2
F	-180.5	-181.1	-181.8	-181.9
H	4.48	4.59	4.76	4.81
iso-Pr	0.28	0.35	0.35	0.34
sec-Bu	0.40	0.43	0.44	0.41
n-Pr	0.15	0.23	0.35	0.38

Optimized cartesian coordinates for compound 6.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.945559	0.356467	-0.667483
2	6	0	-1.281477	1.508191	-0.665497
3	6	0	0.000000	1.398365	0.133799
4	7	0	-0.000000	-0.000181	0.646486
5	6	0	-1.210655	-0.698903	0.131896
6	1	0	-2.892413	0.167402	-1.159193
7	1	0	-1.591404	2.423653	-1.155312
8	1	0	0.000000	2.124814	0.959897
9	1	0	-1.841348	-1.061824	0.957049
10	6	0	1.281477	1.508191	-0.665497
11	1	0	1.591404	2.423653	-1.155312
12	6	0	-0.664759	-1.865010	-0.665234
13	1	0	-1.302438	-2.591475	-1.154795
14	6	0	0.664759	-1.865010	-0.665234
15	1	0	1.302438	-2.591475	-1.154795
16	6	0	1.945559	0.356467	-0.667483
17	1	0	2.892413	0.167402	-1.159193

18	6	0	1.210655	-0.698903	0.131896
19	1	0	1.841348	-1.061824	0.957049

Optimized cartesian coordinates for compound 7.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.941296	0.356472	-0.665734
2	6	0	-1.279001	1.506198	-0.663009
3	6	0	-0.000000	1.439300	0.126805
4	7	0	-0.000000	0.000754	0.700552
5	6	0	-1.245231	-0.717935	0.124779
6	1	0	-2.877774	0.162192	-1.171888
7	1	0	-1.579513	2.415286	-1.167166
8	1	0	-0.000000	2.143229	0.965269
9	1	0	-1.856782	-1.068135	0.962824
10	6	0	1.279001	1.506198	-0.663009
11	1	0	1.579513	2.415286	-1.167166
12	6	0	-0.663489	-1.861799	-0.661052
13	1	0	-1.300414	-2.578281	-1.162960
14	6	0	0.663489	-1.861799	-0.661052
15	1	0	1.300414	-2.578281	-1.162960
16	6	0	1.941296	0.356472	-0.665734
17	1	0	2.877774	0.162192	-1.171888
18	6	0	1.245231	-0.717935	0.124779
19	1	0	1.856782	-1.068135	0.962824
20	6	0	0.000000	-0.002060	2.196296
21	1	0	0.892754	0.512372	2.551095
22	1	0	-0.892754	0.512372	2.551095
23	1	0	0.000000	-1.033964	2.546627

Optimized cartesian coordinates for compound 8.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.054335	0.385428	-0.573453
2	6	0	-1.379496	1.558015	-0.638761
3	6	0	-0.000000	1.470445	-0.005517
4	7	0	-0.000000	0.037533	0.459844
5	6	0	-1.172134	-0.667387	-0.124598
6	1	0	-3.060890	0.226047	-0.933839
7	1	0	-1.787950	2.492084	-1.000583
8	1	0	-0.000000	2.137911	0.867645
9	6	0	1.379496	1.558015	-0.638761

10	1	0	1.787950	2.492084	-1.000582
11	6	0	-0.735880	-1.902095	-0.475261
12	1	0	-1.336056	-2.685097	-0.915168
13	6	0	0.735880	-1.902095	-0.475261
14	1	0	1.336056	-2.685097	-0.915168
15	6	0	2.054335	0.385428	-0.573453
16	1	0	3.060890	0.226047	-0.933839
17	6	0	1.172134	-0.667387	-0.124598
18	6	0	0.000000	-0.063508	1.972704
19	1	0	0.896746	0.431282	2.342926
20	1	0	-0.896746	0.431282	2.342926
21	1	0	0.000000	-1.116213	2.245010

Optimized cartesian coordinates for compound 9.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.067858	0.369766	-0.403471
2	6	0	-1.354051	1.606080	-0.403844
3	6	0	0.000000	1.386656	-0.105754
4	7	0	-0.000000	0.000115	0.379284
5	6	0	-1.200738	-0.693118	-0.105765
6	1	0	-3.100262	0.270926	-0.706405
7	1	0	-1.784713	2.549446	-0.707151
8	6	0	1.354051	1.606080	-0.403844
9	1	0	1.784713	2.549446	-0.707151
10	6	0	-0.713819	-1.975529	-0.403648
11	1	0	-1.315622	-2.820294	-0.706347
12	6	0	0.713819	-1.975529	-0.403648
13	1	0	1.315622	-2.820294	-0.706347
14	6	0	2.067858	0.369766	-0.403471
15	1	0	3.100262	0.270926	-0.706405
16	6	0	1.200738	-0.693118	-0.105765
17	6	0	-0.000000	-0.000185	1.892958
18	1	0	0.898327	0.518334	2.223143
19	1	0	-0.000000	-1.037809	2.221823
20	1	0	-0.898327	0.518334	2.223143

Optimized cartesian coordinates for compound 10.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.354672	-1.927265	-0.857446
2	6	0	-1.510003	-1.261576	-0.841218

3	6	0	-1.579845	0.000000	-0.000542
4	15	0	0.012309	0.000000	1.035408
5	6	0	0.788222	-1.366870	-0.031655
6	1	0	-0.201152	-2.814120	-1.466489
7	1	0	-2.366948	-1.566015	-1.436214
8	1	0	-2.469880	0.000000	0.636339
9	1	0	1.243911	-2.145379	0.588085
10	6	0	-1.510003	1.261576	-0.841218
11	1	0	-2.366948	1.566015	-1.436215
12	6	0	1.832344	-0.666765	-0.881353
13	1	0	2.514734	-1.250066	-1.493845
14	6	0	1.832344	0.666765	-0.881353
15	1	0	2.514734	1.250066	-1.493845
16	6	0	-0.354672	1.927265	-0.857446
17	1	0	-0.201152	2.814120	-1.466489
18	6	0	0.788222	1.366870	-0.031655
19	1	0	1.243911	2.145379	0.588085

Optimized cartesian coordinates for compound 11.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.942658	0.352896	-0.762492
2	6	0	-1.276941	1.509837	-0.759533
3	6	0	-0.000000	1.609334	0.070572
4	15	0	0.000000	0.001279	0.961686
5	6	0	-1.391460	-0.802665	0.068005
6	1	0	-2.832458	0.189492	-1.359818
7	1	0	-1.581149	2.363569	-1.354412
8	1	0	0.000000	2.482322	0.728817
9	1	0	-2.149147	-1.237395	0.725586
10	6	0	1.276941	1.509837	-0.759533
11	1	0	1.581149	2.363569	-1.354412
12	6	0	-0.667404	-1.862274	-0.757412
13	1	0	-1.254490	-2.554651	-1.350039
14	6	0	0.667404	-1.862274	-0.757412
15	1	0	1.254490	-2.554651	-1.350039
16	6	0	1.942658	0.352896	-0.762492
17	1	0	2.832458	0.189492	-1.359818
18	6	0	1.391460	-0.802665	0.068005
19	1	0	2.149147	-1.237395	0.725586
20	6	0	0.000000	-0.002026	2.770377
21	1	0	0.892029	0.512092	3.133707
22	1	0	-0.892029	0.512092	3.133707
23	1	0	-0.000000	-1.032712	3.130693

Optimized cartesian coordinates for compound 12.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.343899	-2.076419	-0.765534
2	6	0	-1.509288	-1.379941	-0.822472
3	6	0	-1.613657	0.000000	-0.116878
4	15	0	-0.023907	0.000000	0.752447
5	6	0	0.771606	-1.307039	-0.188410
6	1	0	-0.225151	-3.038231	-1.250810
7	1	0	-2.388239	-1.782546	-1.313835
8	1	0	-2.499583	0.000000	0.524707
9	6	0	-1.509288	1.379941	-0.822472
10	1	0	-2.388239	1.782546	-1.313835
11	6	0	1.886519	-0.746678	-0.740907
12	1	0	2.524910	-1.256033	-1.455670
13	6	0	1.886519	0.746678	-0.740907
14	1	0	2.524910	1.256033	-1.455670
15	6	0	-0.343899	2.076419	-0.765534
16	1	0	-0.225151	3.038231	-1.250810
17	6	0	0.771606	1.307039	-0.188410
18	6	0	0.045967	0.000000	2.557855
19	1	0	-0.454118	0.893932	2.935735
20	1	0	-0.454118	-0.893932	2.935735
21	1	0	1.091574	0.000000	2.871473

Optimized cartesian coordinates for compound 13.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.060522	0.358515	-0.562322
2	6	0	-1.340660	1.605760	-0.561880
3	6	0	-0.000000	1.551917	-0.078134
4	15	0	0.000000	0.000056	0.769726
5	6	0	-1.343660	-0.775625	-0.078597
6	1	0	-3.002990	0.297300	-1.098969
7	1	0	-1.759051	2.452791	-1.098027
8	6	0	1.340660	1.605760	-0.561880
9	1	0	1.759051	2.452791	-1.098027
10	6	0	-0.719980	-1.963881	-0.562021
11	1	0	-1.244421	-2.750123	-1.097520
12	6	0	0.719980	-1.963881	-0.562021
13	1	0	1.244421	-2.750123	-1.097520
14	6	0	2.060522	0.358515	-0.562322
15	1	0	3.002990	0.297300	-1.098969
16	6	0	1.343660	-0.775625	-0.078597

17	6	0	0.000000	-0.000301	2.581202
18	1	0	0.893531	0.515469	2.935815
19	1	0	0.000000	-1.032086	2.935579
20	1	0	-0.893531	0.515469	2.935815

Optimized cartesian coordinates for compound 14.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.341247	-1.925278	-0.561128
2	6	0	-1.497272	-1.258545	-0.560856
3	6	0	-1.624419	0.000025	0.275223
4	33	0	-0.000154	-0.000004	1.472814
5	6	0	0.811668	-1.405983	0.275249
6	1	0	-0.191119	-2.801348	-1.188082
7	1	0	-2.330982	-1.566988	-1.187686
8	1	0	-2.549754	0.000035	0.857678
9	1	0	1.274162	-2.207412	0.857761
10	6	0	-1.497241	1.258598	-0.560847
11	1	0	-2.330944	1.567063	-1.187677
12	6	0	1.838775	-0.667320	-0.560344
13	1	0	2.523192	-1.235365	-1.186468
14	6	0	1.838791	0.667267	-0.560346
15	1	0	2.523224	1.235293	-1.186470
16	6	0	-0.341191	1.925284	-0.561133
17	1	0	-0.191036	2.801346	-1.188091
18	6	0	0.811704	1.405958	0.275248
19	1	0	1.274220	2.207374	0.857761

Optimized cartesian coordinates for compound 15.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.359900	-1.938057	-0.890848
2	6	0	-1.516904	-1.271243	-0.874591
3	6	0	-1.661135	0.000000	-0.046727
4	33	0	0.011900	0.000000	0.971745
5	6	0	0.828691	-1.437221	-0.079954
6	1	0	-0.217298	-2.816954	-1.510749
7	1	0	-2.361739	-1.580732	-1.480856
8	1	0	-2.562461	0.000000	0.568566
9	1	0	1.290006	-2.225129	0.517920
10	6	0	-1.516904	1.271243	-0.874591
11	1	0	-2.361739	1.580732	-1.480857

12	6	0	1.843253	-0.667759	-0.916271
13	1	0	2.523802	-1.237658	-1.540082
14	6	0	1.843253	0.667759	-0.916271
15	1	0	2.523802	1.237658	-1.540082
16	6	0	-0.359900	1.938057	-0.890848
17	1	0	-0.217298	2.816954	-1.510749
18	6	0	0.828691	1.437221	-0.079954
19	1	0	1.290006	2.225129	0.517919
20	6	0	0.038460	0.000000	2.907840
21	1	0	-0.473429	0.895050	3.261175
22	1	0	-0.473430	-0.895049	3.261175
23	1	0	1.076581	-0.000000	3.239978

Optimized cartesian coordinates for compound 16.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.068108	-0.278751	-0.786494
2	6	0	1.370972	-1.441735	-0.858800
3	6	0	-0.000000	-1.615279	-0.156929
4	6	0	1.342219	0.841599	-0.165078
5	1	0	3.015291	-0.157553	-1.300836
6	1	0	1.776794	-2.297213	-1.389150
7	1	0	-0.000000	-2.556010	0.397582
8	6	0	-1.370972	-1.441735	-0.858800
9	1	0	-1.776794	-2.297213	-1.389150
10	6	0	0.744061	1.921304	-0.740460
11	1	0	1.230503	2.509687	-1.513565
12	6	0	-0.744061	1.921304	-0.740460
13	1	0	-1.230503	2.509687	-1.513565
14	6	0	-2.068108	-0.278750	-0.786494
15	1	0	-3.015291	-0.157553	-1.300836
16	6	0	-1.342219	0.841599	-0.165078
17	6	0	0.000000	0.030093	2.858662
18	1	0	-0.897238	-0.478964	3.209771
19	1	0	0.897238	-0.478964	3.209771
20	1	0	0.000000	1.073507	3.173434
21	33	0	0.000000	-0.004089	0.923610

Optimized cartesian coordinates for compound 17.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.348641	2.038968	-0.716394
2	6	0	1.591961	1.321472	-0.715409
3	6	0	1.597334	0.000001	-0.182433
4	33	0	-0.000764	0.000000	0.849204
5	6	0	-0.798766	1.383329	-0.183600
6	1	0	0.279132	2.928522	-1.338069
7	1	0	2.397742	1.706136	-1.336151
8	6	0	1.591962	-1.321471	-0.715409
9	1	0	2.397744	-1.706134	-1.336151
10	6	0	-1.940386	0.717688	-0.717144
11	1	0	-2.676314	1.223167	-1.337993
12	6	0	-1.940385	-0.717689	-0.717144
13	1	0	-2.676313	-1.223169	-1.337994
14	6	0	0.348643	-2.038968	-0.716394
15	1	0	0.279134	-2.928521	-1.338069
16	6	0	-0.798765	-1.383329	-0.183599
17	6	0	-0.000674	0.000000	2.785382
18	1	0	0.516264	-0.895047	3.129126
19	1	0	-1.034050	-0.000000	3.129818
20	1	0	0.516264	0.895048	3.129126

Optimized cartesian coordinates for compound S1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.305444	2.101894	-0.417458
2	6	0	1.401894	1.318486	-0.637910
3	6	0	1.257840	0.000000	-0.143076
4	7	0	-0.083442	0.000000	0.618810
5	6	0	-0.813542	1.251701	0.140975
6	1	0	0.198847	3.156739	-0.620141
7	1	0	2.304862	1.655711	-1.132680
8	1	0	-1.330098	1.703617	0.996171
9	6	0	1.401895	-1.318486	-0.637909
10	1	0	2.304863	-1.655711	-1.132679
11	6	0	-1.813893	0.664025	-0.839818
12	1	0	-2.424900	1.305700	-1.460840
13	6	0	-1.813893	-0.664025	-0.839818
14	1	0	-2.424900	-1.305700	-1.460840
15	6	0	0.305444	-2.101894	-0.417458
16	1	0	0.198847	-3.156739	-0.620141
17	6	0	-0.813542	-1.251701	0.140975

18	1	0	-1.330098	-1.703618	0.996170
19	6	0	0.198289	-0.000000	2.077679
20	1	0	0.779961	-0.891476	2.307517
21	1	0	0.779961	0.891476	2.307517
22	1	0	-0.742680	-0.000000	2.634923

Optimized cartesian coordinates for compound S2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.342680	-2.069995	-0.737223
2	6	0	-1.453797	-1.294112	-0.832583
3	6	0	-1.464372	0.000000	-0.139916
4	15	0	0.020877	0.000000	0.794012
5	6	0	0.852166	-1.416286	-0.021777
6	1	0	-0.252032	-3.067870	-1.149538
7	1	0	-2.305501	-1.612543	-1.429813
8	1	0	1.383389	-2.098607	0.647523
9	6	0	-1.453797	1.294111	-0.832584
10	1	0	-2.305500	1.612542	-1.429814
11	6	0	1.805061	-0.669051	-0.956547
12	1	0	2.415851	-1.246445	-1.643237
13	6	0	1.805061	0.669051	-0.956547
14	1	0	2.415851	1.246446	-1.643236
15	6	0	-0.342680	2.069996	-0.737223
16	1	0	-0.252032	3.067870	-1.149537
17	6	0	0.852166	1.416287	-0.021777
18	1	0	1.383389	2.098607	0.647523
19	6	0	-0.046875	0.000000	2.615084
20	1	0	-0.591501	0.887853	2.942196
21	1	0	-0.591501	-0.887853	2.942196
22	1	0	0.958525	0.000000	3.041947

Optimized cartesian coordinates for compound S3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.947319	-0.326434	-2.067934
2	6	0	-1.052677	-1.431424	-1.280917
3	6	0	-0.348447	-1.505798	0.000002
4	33	0	0.735575	0.050559	-0.000000
5	6	0	-0.235678	0.892759	-1.469179
6	1	0	-1.381278	-0.253313	-3.059136
7	1	0	-1.688869	-2.258397	-1.593171

8	1	0	0.375263	1.444139	-2.186558
9	6	0	-1.052677	-1.431420	1.280921
10	1	0	-1.688869	-2.258393	1.593177
11	6	0	-1.159475	1.809980	-0.669394
12	1	0	-1.870159	2.411746	-1.228437
13	6	0	-1.159475	1.809982	0.669389
14	1	0	-1.870159	2.411750	1.228431
15	6	0	-0.947319	-0.326429	2.067935
16	1	0	-1.381277	-0.253305	3.059137
17	6	0	-0.235677	0.892763	1.469176
18	1	0	0.375263	1.444145	2.186554
19	6	0	2.680553	-0.102276	0.000000
20	1	0	2.969004	-0.660948	0.890757
21	1	0	2.969004	-0.660950	-0.890755
22	1	0	3.141018	0.885273	-0.000001

Optimized cartesian coordinates for compound 18.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.372320	2.062369	-0.555371
2	6	0	1.600317	1.353347	-0.555609
3	6	0	1.464044	0.000001	-0.270251
4	8	0	0.000096	0.000000	0.284183
5	6	0	-0.731535	1.267391	-0.271558
6	1	0	0.285880	3.094053	-0.864775
7	1	0	2.536951	1.794409	-0.865050
8	6	0	1.600318	-1.353345	-0.555608
9	1	0	2.536952	-1.794407	-0.865050
10	6	0	-1.971955	0.709055	-0.556160
11	1	0	-2.822427	1.299832	-0.864812
12	6	0	-1.971955	-0.709056	-0.556160
13	1	0	-2.822427	-1.299834	-0.864812
14	6	0	0.372321	-2.062369	-0.555371
15	1	0	0.285882	-3.094053	-0.864774
16	6	0	-0.731534	-1.267392	-0.271558
17	6	0	-0.000918	0.000000	1.826923
18	1	0	0.524602	-0.910606	2.097399
19	1	0	-1.052670	0.000000	2.095810
20	1	0	0.524601	0.910607	2.097399

Optimized cartesian coordinates for compound 19.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.368342	2.066147	-0.663971
2	6	0	1.605615	1.352002	-0.663359
3	6	0	1.558551	0.000001	-0.218417
4	16	0	-0.000198	0.000000	0.607990
5	6	0	-0.779098	1.349510	-0.219091
6	1	0	0.296133	3.033552	-1.145995
7	1	0	2.479786	1.773156	-1.144912
8	6	0	1.605616	-1.352001	-0.663360
9	1	0	2.479788	-1.773154	-1.144912
10	6	0	-1.973526	0.714226	-0.664327
11	1	0	-2.775331	1.260702	-1.145899
12	6	0	-1.973526	-0.714227	-0.664327
13	1	0	-2.775330	-1.260704	-1.145899
14	6	0	0.368343	-2.066147	-0.663971
15	1	0	0.296135	-3.033552	-1.145995
16	6	0	-0.779097	-1.349510	-0.219091
17	6	0	-0.000808	0.000000	2.410896
18	1	0	0.521764	-0.905399	2.719934
19	1	0	-1.046311	0.000000	2.719570
20	1	0	0.521764	0.905400	2.719934

Optimized cartesian coordinates for Me_4O^{2+}.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.000000
2	6	0	0.928361	0.928361	0.928361
3	1	0	0.222146	1.513055	1.513055
4	1	0	1.513055	0.222146	1.513055
5	1	0	1.513055	1.513055	0.222146
6	6	0	-0.928361	-0.928361	0.928361
7	1	0	-1.513055	-0.222146	1.513055
8	1	0	-1.513055	-1.513055	0.222146
9	1	0	-0.222146	-1.513055	1.513055
10	6	0	-0.928361	0.928361	-0.928361
11	1	0	-0.222146	1.513055	-1.513055
12	1	0	-1.513055	0.222146	-1.513055
13	1	0	-1.513055	1.513055	-0.222146
14	6	0	0.928361	-0.928361	-0.928361
15	1	0	1.513055	-0.222146	-1.513055
16	1	0	1.513055	-1.513055	-0.222146
17	1	0	0.222146	-1.513055	-1.513055