Binuclear Chromium Carbonyl Complexes of Methylaminobis(difluorophosphine): Metal-Metal Bonds Versus Four-Electron Donor Bridging Carbonyl Groups

Huijuan Miao,[a,b] Xiuhui Zhang,*[a,b] Yang Bai,[a,b] Qian-shu Li[b,c] and R. Bruce King*[c,d]

[a] Key Laboratory of Cluster Science, Ministry of Education of China, School of Chemistry, Beijing Institute of Technology, Beijing 100081, P. R. China

[b] State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, PR China

[c] MOE Key Laboratory of Theoretical Chemistry of Environment, Center for Computational Quantum Chemistry, South China Normal University, Guangzhou 510006, PR China

[d] Department of Chemistry and Center for Computational Chemistry, University of Georgia, Athens, Georgia 30606, USA

Supporting Information

Tables S1 to S10: Energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), and numbers of imaginary vibrational frequencies (Nimg) for the twelve optimized $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) structures using the M06-L/TZP method.

Tables S11 to S18: Infrared active ν(CO) frequencies (cm^{-1}) predicted for $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) structures at the M06-L /TZP level.

Tables S19 to S40: Atomic coordinates for $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) structures at the M06-L /TZP levels.

Tables S41 to S54: Energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), and numbers of imaginary vibrational frequencies (Nimg) for the 26 optimized $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) structures using the B3LYP/DZP and BP86/DZP methods.

Figures S1 to S9: Optimized structures for $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4; and m=3, n=6, 5, 4) by the B3LYP/DZP and BP86/DZP methods.

Tables S55 to S63: Infrared active ν(CO) frequencies (cm^{-1}) predicted for $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) structures at the B3LYP/DZP and BP86/DZP levels;

Tables S64 to S99: Atomic coordinates for $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) structures at the B3LYP/DZP and BP86/DZP levels.

Tables S100 to S108: Atomic coordinates for the lowest-energy open-shell singlet structures of $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) at the M06-L/TZP level.

Tables S109 to S111: Total energies (E, in kcal mol^{-1}) and numbers of imaginary vibrational frequencies (Nimg) for the open-shell singlet structures of $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8; m=2, n=8, 7, 6; and m=3, n=6, 5, 4) using the M06-L /TZP method.

Figures S10 to S13: The frontier molecular orbital graphs of the unpaired electrons in the four open-shell triplet structures.

Table S1: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the one singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_{10}$ using M06-L/TZP method.

Singlet		**110-1S(C_1)**
M06-L	E	-4399.819755
	ΔE	0.0
	Nimg	0

Table S2: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_9$ using M06-L/TZP method.

Singlet		**19-1S(C_1)**	**19-2S(C_1)**
M06-L	E	-4286.423658	-4286.421063
	ΔE	0.0	1.6
	Nimg	0	0

Table S3: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_8$ using M06-L/TZP method.

Singlet		**18-1S(C_1)**	**18-2S(C_1)**	**18-3S(C_1)**
M06-L	E	-4173.044978	-4173.043969	-4173.043458
	ΔE	0.0	0.6	1.0
	Nimg	0	0	0

Table S4: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) spin expectation values (S^2) for the two triplet stationary points of $MeN(PF_2)_2Cr_2(CO)_8$ using M06-L/TZP method.

Triplet		**18-1T(C_1)**	**18-2T (C_S)**
M06-L	E	-4173.029702	-4173.020606
	ΔE	9.6	15.3
	$<S^2>$	2.07	2.07
	Nimg	0	0

Table S5: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_8$ and $[MeN(PF_2)_2]_2Cr_2(CO)_7$ using M06-L/TZP method.

Singlet		**28-1S(C_S)**	**27-1S(C_1)**
M06-L	E	-5350.126305	-5236.756710
	ΔE	0.0	0.0
	Nimg	0	0

Table S6: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_6$ using M06-L/TZP method.

Singlet		**26-1S(C_S)**	**26-2S(C_1)**
M06-L	E	-5123.382333	-5123.381113
	ΔE	0.0	0.8
	Nimg	0	0

Table S7: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_6$ using M06-L/TZP method.

Singlet		**36-1S(C_1)**	**36-2S(C_1)**	**36-3S(C_1)**
M06-L	E	-6300.45795	-6300.453207	-6300.422173
	ΔE	0.0	3.0	22.4
	Nimg	0	0	0

Table S8: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_5$ using M06-L/TZP method.

Singlet		**35-1S(C_1)**	**35-2S(C_1)**	**35-3S(C_1)**
M06-L	E	-6187.096022	-6187.086847	-6187.083224
	ΔE	0.0	5.8	8.0
	Nimg	0	0	0

Table S9: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_4$ using M06-L/TZP method.

Singlet		**34-1S(C_1)**	**34-2S(C_1)**
M06-L	E	-6073.729736	-6073.703794
	ΔE	0.0	16.3
	Nimg	0	0

Table S10: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) spin expectation values (S^2) for the two triplet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_4$ using M06-L/TZP method.

Triplet		**34-1T(C_1)**	**34-2T (C_1)**
M06-L	E	-6073.706269	-6073.693914
	ΔE	14.7	22.5
	$<S^2>$	2.07	2.06
	Nimg	0	0

Table S11: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the one singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_{10}$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
110-1S(C_1)	2023(1850),2039(170),2046(1188),2048(2344),2061(869), 2072(738),2075(542),2076(241),2144(501),2151(105)

Table S12: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_9$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
19-1S(C_1)	1946(1654),2016(760),2028(818),2052(709),2065(2076), 2073(769),2084(353),2119(540),2150(302)
19-2S(C_1)	1950(231),2023(359),2037(800),2046(986),2058(431), 2061(1295),2068(949),2099(1490),2139(375)

Table S13: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points and two triplet stationary points of $MeN(PF_2)_2Cr_2(CO)_8$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
18-1S(*C*$_1$)	1961(240,1985(1143),2030(509),2043(230),2058(1347),2070(731),2097(1898),2133(444)
18-2S(*C*$_1$)	1880(364),1945(305),2032(653),2036(747),2060(605),2073(1348),2083(1634),2131(662)
18-3S(*C*$_1$)	2021(769),2037(110),2062(720),2075(2176),2080(484),2087(275),2115(1703),2151(16)
18-1T(*C*$_1$)	1994(90),2014(699),2043(1072),2049(386),2051(3558),2059(821),2061(999),2130(443)
18-2T(*C*$_S$)	2030(887),2053(1656),2060(639),2064(989),2084(2606),2094(1591),2104(364),2146(158)

Table S14: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_8$ and $[MeN(PF_2)_2]_2Cr_2(CO)_7$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
28-1S(*C*$_S$)	2011(128),2028(698),2032(1985),2048(133),2055(2244),2072(241),2119(795),2130(1)
27-1S(*C*$_1$)	1900(254),2017(376),2042(572),2047(1088),2056(1491),2083(1469),2114(23)

Table S15: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_6$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
26-1S(*C*$_S$)	1943(1),1967(1076),2039(180),2040(1583),2085(1838),2106(1)
26-2S(*C*$_1$)	1857(3360,1913(3570,2037(547),2047(1434),2066(1706),2101(295)

Table S16: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_6$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
36-1S(*C*$_1$)	2031(640), 2039(385), 2042(705), 2043 (1134), 2088(2299), 2099(76)
36-2S(*C*$_1$)	2010(143), 2027(1451), 2036(1124), 2047(1395), 2092(206), 2099(114)
36-3S(*C*$_1$)	1985(137), 1997(1692), 2036(590), 2037(613), 2080(1743), 2090(98)

Table S17: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_5$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
35-1S(*C_1*)	1878(233), 2037(770), 2042(610), 2061(1960), 2085(536)
35-2S(*C_1*)	2003(713), 2037(487), 2045(908), 2050(1118), 2097(951)
35-3S(*C_1*)	1871(346), 1993(549), 2040(1735), 2052(437), 2087(844)

Table S18: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points and two triplet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_4$ at M06-L/TZP level.(infrared intensities in parentheses are in km mol^{-1}).

	M06-L
34-1S(*C_1*)	2014(718), 2058(794), 2074(1757), 2095(361)
34-2S(*C_1*)	2020(1721), 2021(40), 2052(1927), 2073(256)
34-1T(*C_1*)	2011(441), 2044(3096), 2045(677), 2082(464)
34-2T(*C_1*)	2043(1158), 2047(801), 2066(2310), 2090(275)

Table S19: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_{10}$ structure **110-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-0.045113	-1.010256	0.707261
15	-1.665766	-1.289233	0.225548
15	1.224759	-0.823122	-0.387907
24	3.180544	0.274904	0.040559
24	-3.087798	0.437599	-0.065131
9	0.390675	-0.319755	-1.650456
9	1.394997	-2.307395	-0.911044
9	-1.405598	-2.287458	-0.96291
9	-2.060148	-2.359807	1.323915
6	3.580198	-0.956844	1.440614
6	2.407483	1.504112	1.280081
6	4.854558	1.125361	0.287519
6	2.748614	1.500029	-1.367378
6	4.005098	-0.892752	-1.229884
6	-1.576424	1.587331	-0.025574
6	-3.262124	0.574118	1.827993
6	-4.538263	-0.812205	-0.108475
6	-2.883069	0.269818	-1.964516
6	-4.275681	1.906843	-0.298601
8	3.821154	-1.695059	2.283719
8	2.480566	2.231183	-2.203677
8	5.868693	1.63459	0.435848
8	4.511655	-1.580249	-1.990163
8	1.976453	2.264929	2.020052
8	-4.987539	2.791153	-0.435601
8	-5.396001	-1.568283	-0.129469
8	-2.743305	0.161866	-3.093197
8	-3.351758	0.646765	2.967996
8	-0.617898	2.217135	0.007389
6	0.092753	-0.541421	2.092989
1	-0.427192	-1.222777	2.764895
1	1.142475	-0.537126	2.374411
1	-0.304664	0.468091	2.227659

Table S20: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **19-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-0.091653	2.165809	0.017116
15	-1.596558	1.448992	0.065628
15	1.44368	1.395912	-0.029052
24	-2.214565	-0.759097	0.038278
24	2.252895	-0.705221	0.066564
6	-0.091512	3.641862	-0.140316
1	0.811749	4.049626	0.304275
1	-0.132583	3.914367	-1.193458
1	-0.948769	4.066362	0.376856
9	-2.308273	2.27808	-1.090953
9	-2.260314	2.272952	1.252282
9	2.147595	2.34766	1.03518
9	1.974983	2.183644	-1.3066
6	3.825773	0.1799	-0.257499
6	1.953917	-0.876608	-1.813335
6	2.516193	-0.49587	1.952634
6	3.304074	-2.288621	0.074632
6	-1.886466	-0.785946	-1.849751
6	-3.995902	-0.085214	-0.271526
6	-2.511904	-0.674819	1.927728
6	-2.928595	-2.512869	-0.031018
8	4.824645	0.721014	-0.458061
8	2.714313	-0.339945	3.069628
8	1.819087	-0.939638	-2.949974
8	4.003013	-3.195204	0.062553
8	-2.67856	-0.623498	3.05689
8	-5.056483	0.295404	-0.452316
8	-1.685553	-0.806232	-2.974637
8	-3.357248	-3.572413	-0.072073
6	-0.537146	-1.500327	0.350417
8	0.467775	-2.048355	0.551325

Table S21: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **19-2S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
15	-1.302459	1.56024	0.473252
15	1.373986	1.495216	-0.503359
24	1.560795	-0.676692	0.160388
24	-1.545814	-0.624235	-0.110693
6	0.3079	-1.361447	-1.322781
8	0.272938	-1.896196	-2.349317
6	0.901395	-0.091853	1.869863
6	2.725824	-1.017609	-1.300023
6	-1.81156	0.078344	-1.863606
6	-2.022773	-2.362386	-0.700102
6	1.517122	-2.477069	0.770127
6	-1.506777	-1.364569	1.661454
6	3.217827	-0.381371	0.994373
6	-3.361513	-0.352627	0.151894
8	0.696419	0.28664	2.932325
8	4.236007	-0.203082	1.487314
8	1.461939	-3.554914	1.148105
8	3.463036	-1.197774	-2.155232
8	-1.581995	-1.841404	2.699517
8	-4.489285	-0.194478	0.306808
8	-2.038683	0.501385	-2.904053
8	-2.374304	-3.394115	-1.050108
9	-1.567309	2.087704	1.943185
9	-2.36224	2.52618	-0.209526
9	2.570472	2.468884	-0.144038
9	1.355942	1.836332	-2.052921
7	0.100597	2.419491	0.082172
6	0.102715	3.888934	0.040327
1	-0.166209	4.25442	-0.951277
1	-0.61919	4.266154	0.76182
1	1.087454	4.262928	0.310831

Table S22: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **18-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	0.006292	2.432739	0.028583
15	1.433927	1.548	0.042322
15	-1.425078	1.555671	-0.01614
6	0.011191	3.901492	-0.027109
1	-0.893498	4.286413	0.439436
1	0.870531	4.283912	0.520369
1	0.058773	4.248067	-1.05915
9	-2.172564	2.316917	-1.192306
9	-2.226264	2.281049	1.144466
9	2.218769	2.287867	-1.120827
9	2.204915	2.287185	1.216973
24	1.390847	-0.725491	-0.019532
24	-1.394752	-0.719857	0.016448
6	-0.422605	-0.64831	1.665915
6	-2.835799	-0.702729	1.176016
6	1.451497	-2.623381	-0.063165
6	-1.464682	-2.617325	0.025702
6	-2.708667	-0.710266	-1.384688
6	0.418978	-0.612135	-1.666465
6	2.833204	-0.698429	-1.177429
6	2.702393	-0.742488	1.384191
8	3.715413	-0.686864	-1.914187
8	3.522137	-0.744868	2.179421
8	0.104447	-0.516559	-2.774808
8	1.574074	-3.760037	-0.121552
8	-1.592183	-3.754435	0.062571
8	-3.530261	-0.699829	-2.178051
8	-3.717301	-0.697361	1.913662
8	-0.108282	-0.583799	2.776442

Table S23: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **18-2S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
15	-1.509209	1.508127	-0.024891
15	1.377424	1.602111	-0.065363
24	-1.428889	-0.761803	-0.142058
24	1.477406	-0.669143	-0.158865
6	3.161692	-0.516134	-0.952321
6	2.407052	-0.679733	1.43434
6	-1.405689	-2.662237	-0.203747
6	1.648688	-2.55825	-0.186644
6	-0.109537	-0.700325	1.472832
6	-0.238453	-0.673665	-1.584751
6	-2.669316	-0.859958	1.320749
6	-2.938081	-0.730455	-1.268065
8	-3.402383	-0.915786	2.19338
8	-3.84412	-0.704845	-1.967819
8	0.624331	-0.628795	-2.375973
8	-1.424935	-3.804311	-0.253817
8	1.836639	-3.688373	-0.154525
8	-0.07204	-0.656723	2.630259
8	2.998289	-0.689202	2.419732
8	4.201332	-0.424103	-1.429749
9	2.0534	2.458411	-1.221115
9	2.158701	2.319821	1.111343
9	-2.287528	2.290333	-1.165019
9	-2.31828	2.166888	1.169884
7	-0.099517	2.412742	0.039532
6	-0.154308	3.883155	0.057627
1	0.753934	4.272406	0.512784
1	-0.246294	4.279109	-0.953439
1	-1.004479	4.212083	0.652024

.

Table S24: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **18-3S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
15	-0.619272	1.914924	0.010201
24	-1.521821	-0.243954	0.043822
24	1.522572	-0.040848	0.00078
6	-1.577227	-0.246109	-1.862984
6	-3.207661	0.647328	0.046551
6	-2.547235	-1.81432	0.209858
6	-1.377856	-0.102488	1.940298
6	1.630415	-0.285091	1.908818
6	3.300664	0.644624	0.071752
6	1.392023	0.387264	-1.879309
6	2.481901	-1.576211	-0.378328
15	0.094919	-1.769875	-0.083544
8	-1.621916	-0.247305	-3.005388
8	-4.227419	1.158868	0.038239
8	-3.174452	-2.7667	0.325615
8	1.358063	0.644454	-2.990187
8	3.117636	-2.509387	-0.613132
8	-1.313859	-0.002315	3.07791
8	1.754486	-0.430914	3.033322
8	4.37962	1.012606	0.112383
9	-1.43026	2.972073	0.889061
9	-0.871998	2.697733	-1.366694
9	0.241495	-2.894815	1.015749
9	0.126348	-2.750706	-1.320537
7	0.901608	1.996682	0.424263
6	1.723871	3.186766	0.433398
1	2.22069	3.356888	-0.528848
1	1.134793	4.078107	0.661705
1	2.499619	3.104104	1.19839

Table S25: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **18-1T** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
15	1.274137	1.456439	-0.535526
15	-1.238992	1.460563	0.547584
24	1.329246	-0.682846	0.227527
24	-1.33959	-0.667244	-0.229621
6	-3.198392	-0.646523	0.124901
6	-1.486346	0.056771	-2.01403
6	1.374513	-2.506055	0.862241
6	-1.419058	-2.483865	-0.881417
6	1.071647	-1.28436	-1.564651
6	-1.096513	-1.286877	1.559131
6	3.188379	-0.699696	-0.127975
6	1.486163	0.021656	2.018897
8	4.312225	-0.714591	-0.346629
8	1.586024	0.45334	3.07389
8	-1.077555	-1.645883	2.652386
8	1.414618	-3.592295	1.214304
8	-1.478753	-3.565705	-1.243947
8	1.046873	-1.636467	-2.660263
8	-1.580809	0.502091	-3.063905
8	-4.322543	-0.63854	0.34262
9	-1.254203	1.745963	2.106021
9	-2.440087	2.444545	0.205189
9	2.502535	2.406154	-0.196634
9	1.285754	1.752917	-2.092169
7	0.0275	2.430751	0.019198
6	-0.003615	3.894063	-0.008576
1	1.012656	4.273233	-0.089768
1	-0.591912	4.256054	-0.85185
1	-0.439442	4.27008	0.916148

Table S26: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **18-2T** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-0.954503	1.758755	0.000019
15	0.68731	1.791838	0
24	1.874648	-0.191986	0.000002
24	-1.923352	-0.015027	0.000001
9	1.039388	2.819941	-1.170832
9	1.039416	2.819956	1.17081
6	-1.655602	3.037913	0.000029
1	-2.294164	3.125506	0.883059
1	-0.971787	3.88829	0.000052
1	-2.294141	3.125535	-0.883014
6	1.80218	-0.189525	1.901526
6	3.543092	0.743214	0.000009
6	2.770166	-1.860235	0.000004
6	1.802196	-0.189521	-1.901523
6	-1.837949	-0.086013	-1.960006
6	-3.672596	0.799131	0.000001
6	-1.837964	-0.086042	1.960008
6	-2.772139	-1.768588	-0.000014
15	-0.013555	-1.440029	-0.000006
9	-0.145009	-2.511025	1.184985
9	-0.145007	-2.511012	-1.18501
8	1.728167	-0.193941	3.04562
8	4.551148	1.283997	0.000014
8	3.279907	-2.886261	0.000006
8	-1.769824	-0.131736	3.094651
8	-3.221609	-2.816109	-0.000022
8	1.728193	-0.193933	-3.045618
8	-1.769796	-0.131691	-3.094649
8	-4.731586	1.2294	-0.000001

Table S27: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_8$ structure **28-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
15	0.00199	-1.887012	-2.200432
15	0.002413	1.173913	-2.093687
24	0.018761	-2.14246	0
24	0.004045	2.314686	0
15	0.002413	1.173913	2.093687
15	0.00199	-1.887012	2.200432
6	-1.243833	-3.57098	0
6	1.298394	-3.556892	0
6	-1.503187	-1.020228	0
6	-1.908723	2.363388	0
6	1.536707	-1.010963	0
6	0.010655	3.732249	1.212716
6	1.917915	2.358719	0
8	0.016885	4.657793	1.893144
8	3.054979	2.480166	0
8	2.551765	-0.470931	0
8	-3.046317	2.483637	0
8	-2.518105	-0.479429	0
8	-1.976217	-4.449491	0
8	2.040106	-4.427479	0
6	0.010655	3.732249	-1.212716
8	0.016885	4.657793	-1.893144
9	-1.160814	-2.559479	-3.048094
9	1.184536	-2.514368	-3.055937
9	-1.150099	1.83383	-2.971864
9	1.215508	1.771994	-2.934896
9	-1.160814	-2.559479	3.048094
9	1.184536	-2.514368	3.055937
9	-1.150099	1.83383	2.971864
9	1.215508	1.771994	2.934896
7	-0.050637	-0.346957	-2.874537
7	-0.050637	-0.346957	2.874537
6	-0.181276	-0.294976	4.351713
1	-1.230255	-0.287874	4.642481
1	0.309524	-1.161116	4.789413
1	0.305281	0.598686	4.733256
6	-0.181276	-0.294976	-4.351713
1	0.309524	-1.161116	-4.789413
1	-1.230255	-0.287874	-4.642481
1	0.305281	0.598686	-4.733256

Table S28: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **27-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	3.020293	0.398668	0.067227
15	2.421334	-1.137386	0.417559
15	1.948625	1.608376	-0.416423
24	0.253563	-1.476669	0.011126
24	-0.267604	1.492889	0.000127
7	-3.035845	-0.411582	0.054369
15	-2.432955	1.11087	0.418922
15	-1.950898	-1.62239	-0.419054
9	3.468128	-2.020306	-0.383295
9	3.086973	-1.382318	1.835049
9	2.433579	1.861844	-1.906426
9	2.725465	2.849557	0.198117
9	-2.460508	-1.898215	-1.897033
9	-2.714927	-2.857952	0.222918
9	-3.50031	2.010831	-0.334863
9	-3.050433	1.338201	1.862046
6	-4.476721	-0.697718	0.138478
1	-4.713512	-1.225346	1.061861
1	-5.033934	0.235803	0.106401
1	-4.782689	-1.306521	-0.710861
6	4.463505	0.680034	0.136313
1	4.769331	1.274394	-0.723373
1	4.709346	1.218324	1.051
1	5.014669	-0.257263	0.113988
6	-0.093406	-2.3259	1.669709
6	0.146852	0.173054	1.544189
6	0.519966	-3.246027	-0.476397
6	0.787151	-1.203044	-1.803063
6	-0.732573	0.97418	-1.786783
6	-0.546364	3.185197	-0.746713
6	-0.085483	2.591867	1.526808
8	-0.721098	4.229797	-1.187484
8	0.005613	3.295431	2.424516
8	-1.093543	0.83915	-2.867635
8	0.692048	-4.344028	-0.770791
8	-0.27333	-2.916773	2.634385
8	0.322998	0.146759	2.696346
8	1.18003	-1.192206	-2.881734

Table S29: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **26-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-3.137778	-0.001188	0.011726
15	-2.247438	-1.4251	-0.00724
15	-2.248248	1.423583	0.010728
24	0.000001	-1.377731	0.014823
24	0	1.378471	0.00391
7	3.137779	-0.001187	0.011726
15	2.248248	1.423583	0.010724
15	2.247439	-1.4251	-0.007237
9	-3.028967	-2.247957	1.104573
9	-2.945801	-2.162038	-1.228199
9	-2.954331	2.185796	1.210966
9	-3.02619	2.219629	-1.123753
9	3.028967	-2.247954	1.10458
9	2.945804	-2.162041	-1.228193
9	2.954333	2.185801	1.210959
9	3.026188	2.219626	-1.123761
6	4.604063	0.00176	-0.062136
1	4.938978	0.04147	-1.098536
1	4.995116	0.864347	0.47435
1	4.994012	-0.900299	0.405496
6	-4.604062	0.001759	-0.062137
1	-4.995115	0.864344	0.474354
1	-4.938977	0.041473	-1.098537
1	-4.994011	-0.900302	0.405491
6	0.000002	-2.84816	-1.103234
6	0.000002	-0.449774	-1.649419
6	0	-2.656173	1.444505
6	0	2.666122	-1.415934
6	0.000002	0.447936	1.668229
6	0.000001	2.842879	1.129277
8	-0.000007	0.154253	2.788686
8	0	3.740136	1.849808
8	-0.000004	3.474939	-2.223496
8	-0.000002	-3.458795	2.257968
8	0	-3.749199	-1.81913
8	-0.000004	-0.151646	-2.768894

Table S30: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **26-2S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
15	2.255607	1.429103	-0.083856
15	2.244847	-1.451489	-0.059269
15	-2.241957	-1.452064	-0.100615
15	-2.250268	1.430918	-0.107893
24	0.002002	-1.432268	-0.103058
24	0.002363	1.425246	-0.100091
6	-0.010116	-2.601477	1.415329
8	-0.018142	-3.298247	2.31981
6	-0.002113	2.423968	1.447174
6	0.005232	3.108537	-0.926287
8	-0.005467	3.051805	2.410187
8	0.005764	4.148144	-1.412266
6	0.016706	-0.283243	-1.562973
8	0.025835	0.589556	-2.349767
6	-0.036578	0.002784	1.500798
8	-0.072112	-0.025507	2.663552
6	0.012224	-2.977135	-1.156261
8	0.01871	-3.913214	-1.820467
9	2.984663	-2.244756	1.101055
9	3.013485	-2.193893	-1.234982
9	2.987355	2.23366	1.069364
9	3.039737	2.148575	-1.266146
9	-2.984145	-2.202493	-1.287619
9	-3.008961	-2.235544	1.048761
9	-3.018971	2.178299	-1.282583
9	-2.998131	2.207796	1.054646
7	3.117329	-0.014966	-0.023179
7	-3.112385	-0.014371	-0.084145
6	-4.580539	-0.024491	-0.010236
1	-4.913653	-0.049678	1.026996
1	-4.975455	0.868065	-0.491676
1	-4.968614	-0.896698	-0.532963
6	4.586457	-0.025591	-0.071737
1	4.93995	-0.090682	-1.100624
1	4.970258	0.886277	0.381265
1	4.965074	-0.875611	0.492636

Table S31: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ structure **36-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
24	2.276287	0.058011	-0.45661
24	-2.29987	0.312926	0.342112
7	0.032896	2.79014	-0.52768
15	-1.21258	1.751849	-1.02935
15	1.391175	2.065026	0.131207
9	1.22223	2.408657	1.680657
9	2.41353	3.247413	-0.15546
9	-2.16591	2.895706	-1.57452
9	-0.69341	1.284091	-2.46156
7	0.592712	-0.92381	2.502645
15	-0.99495	-0.81878	1.89925
15	2.024602	-0.71583	1.644786
9	2.709415	-2.12145	1.93701
9	2.840388	0.065166	2.76318
9	-1.3139	-2.38335	1.843715
9	-1.6644	-0.56976	3.321973
6	0.730596	-1.46605	3.877947
1	0.519072	-0.69133	4.611958
1	0.046641	-2.30007	4.022674
1	1.744817	-1.82688	4.022683
7	-0.69116	-1.95085	-1.83985
15	0.904582	-1.60189	-1.35772
15	-2.11027	-1.32843	-1.19245
9	-2.86028	-2.68673	-0.84799
9	-2.89211	-1.08138	-2.55481
9	1.204117	-2.9879	-0.61917
9	1.560631	-2.01546	-2.74705
6	-0.8498	-3.04037	-2.83447
1	-0.63543	-2.67273	-3.83597
1	-0.17852	-3.8637	-2.59842
1	-1.86979	-3.41272	-2.80137
6	-0.1762	4.2479	-0.45084
1	-1.12923	4.478214	0.022377
1	0.618651	4.689124	0.144155
1	-0.15622	4.690035	-1.44607
6	-3.595	-0.66507	1.289693
6	3.499406	-1.3126	-0.83984
8	-4.44583	-1.22815	1.814253
8	4.316677	-2.09178	-1.04351
6	-3.82606	0.917612	-0.55714
8	-4.79888	1.249695	-1.06666
6	2.439185	0.780942	-2.19137
8	2.54277	1.235682	-3.23926
6	3.854273	0.894628	0.092698
8	4.86011	1.346338	0.411873
6	-2.37376	1.747735	1.557635
8	-2.40386	2.637771	2.28384

Table S32: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ structure **36-2S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-0.08821	-2.6037	0.026317
15	-1.68207	-2.06339	-0.14594
15	1.379819	-1.74345	0.097562
9	-2.15703	-3.16911	-1.1896
9	-2.31164	-2.80909	1.122377
9	2.165672	-2.69654	-0.91886
9	1.943525	-2.45055	1.416994
6	0.055493	-4.08261	0.079308
1	0.145755	-4.49304	-0.92479
1	0.935818	-4.34662	0.657329
1	-0.81388	-4.51367	0.56924
7	5.233856	0.814341	0.19533
15	4.281752	-0.57385	0.187406
15	3.919572	1.843198	0.001682
9	4.827683	-1.37648	1.438302
9	4.997178	-1.48456	-0.89284
9	4.35607	2.767058	-1.20943
9	4.163828	2.949551	1.10989
7	-4.8431	1.398654	0.702015
15	-3.62771	1.895364	-0.35559
15	-4.24237	-0.16132	0.886736
9	-4.23491	-0.36127	2.457271
9	-5.51415	-1.06881	0.633787
9	-3.14168	3.259982	0.280182
9	-4.44346	2.569993	-1.53348
24	2.274037	0.376109	-0.01208
24	-2.45989	0.000931	-0.45367
6	6.669348	1.027912	0.255211
1	7.125426	0.278176	0.900881
1	7.121729	0.965028	-0.73584
1	6.873277	2.012015	0.675317
6	-5.96959	2.095535	1.301645
1	-6.8023	1.405141	1.432474
1	-5.70187	2.517624	2.271474
1	-6.29185	2.900851	0.642622
6	-1.22821	0.544671	-1.77905
6	0.998206	1.764763	-0.16875
6	2.133232	0.48514	1.882191
6	2.378998	0.205349	-1.90657
8	0.324485	2.691621	-0.24769
8	-0.55712	0.878224	-2.64898
8	2.491809	0.09517	-3.04172
8	2.089431	0.552889	3.025519
6	-3.54415	-0.65195	-1.86669
6	-1.47597	0.550471	1.072955
8	-4.21606	-1.05608	-2.70363
8	-0.96357	0.863791	2.053115

Table S33: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ structure **36-3S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-0.60871	-2.15655	-1.68391
15	-2.11219	-1.65494	-1.08499
15	0.811312	-1.2063	-1.62565
24	-2.02841	0.232335	0.071268
24	2.033596	0.198478	-0.08927
7	0.025619	3.050279	-0.01978
15	1.373878	2.26494	-0.71438
15	-1.35402	2.311408	0.647473
9	-2.95527	-1.64268	-2.43199
9	-2.65631	-3.06577	-0.60171
9	0.823887	-0.62809	-3.10638
9	1.795334	-2.41571	-1.94572
9	-2.42171	3.402477	0.195284
9	-1.26311	2.828268	2.143494
9	1.250596	2.736707	-2.22168
9	2.448511	3.368471	-0.31621
6	0.123129	4.524329	0.089748
1	0.766519	4.808672	0.921464
1	0.529389	4.93593	-0.83237
1	-0.86579	4.944753	0.240387
6	-0.58821	-3.33371	-2.58086
1	-0.15345	-3.07289	-3.54509
1	-0.01327	-4.14329	-2.13547
1	-1.60677	-3.67467	-2.74752
6	-3.24943	0.036494	1.5225
6	1.38356	0.874023	1.545446
6	-3.60108	0.855931	-0.68391
6	3.248501	-0.04925	-1.53836
6	-1.37725	0.85012	-1.58777
6	3.613891	0.829852	0.644456
8	-1.21183	1.310237	-2.63271
8	4.616954	1.19078	1.073247
8	4.071811	-0.11122	-2.33365
8	-4.60046	1.211088	-1.12591
8	-4.07564	0.003908	2.316585
8	1.208946	1.378512	2.568567
7	0.582896	-2.10552	1.747681
15	-0.82628	-1.141	1.652416
15	2.092504	-1.65116	1.12882
9	-1.82519	-2.33165	1.997898
9	-0.84264	-0.52618	3.118432
9	2.610316	-3.08635	0.69035
9	2.940632	-1.60965	2.472124
6	0.544879	-3.25477	2.679297
1	1.558872	-3.60184	2.860593
1	0.109283	-2.96002	3.633258
1	-0.03742	-4.07096	2.255972

Table S34: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ structure **35-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	2.824176	1.211058	0.447939
15	1.468169	2.086693	-0.04702
15	2.629824	-0.41288	0.848312
24	-0.60771	1.384916	0.41806
24	0.636753	-1.35934	0.468034
7	-2.79007	-1.18377	0.609963
15	-1.45313	-2.06923	0.086836
15	-2.57316	0.455442	0.936828
9	1.881559	3.506519	0.534233
9	1.893289	2.441215	-1.54358
9	3.259637	-0.43094	2.303372
9	3.915204	-1.00968	0.137726
9	-3.12743	0.530077	2.421217
9	-3.89435	1.025841	0.270958
9	-1.85132	-3.47923	0.699959
9	-1.92187	-2.44451	-1.39497
6	-4.14369	-1.75593	0.586255
1	-4.63862	-1.53857	-0.36125
1	-4.08634	-2.83271	0.724877
1	-4.73153	-1.33463	1.400157
6	0.074264	0.056129	1.973487
6	-1.40639	2.980634	-0.0997
6	-0.52843	2.40217	1.987586
6	1.436582	-2.97314	0.008253
6	0.574188	-2.3068	2.081506
8	0.558469	-2.94066	3.036557
8	1.944161	-3.9787	-0.22312
8	-0.50767	3.077243	2.913593
8	0.119825	0.098203	3.140105
8	-1.90869	3.980701	-0.36491
7	-0.09633	-0.09821	-2.69406
15	-1.02703	0.936049	-1.77007
15	0.938491	-1.02133	-1.75672
9	-1.0097	2.202367	-2.72914
9	-2.49534	0.486391	-2.20444
9	2.361203	-0.53711	-2.29179
9	0.921384	-2.33821	-2.64518
6	-0.23595	-0.25788	-4.143
1	-0.85409	-1.12608	-4.37326
1	-0.69665	0.634443	-4.56137
1	0.74545	-0.38551	-4.59721
6	4.174097	1.784864	0.347326
1	4.625422	1.544075	-0.616
1	4.119678	2.864755	0.460674
1	4.800365	1.386504	1.144045

Table S35: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ structure **35-2S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-2.77988	1.618959	-0.85231
15	-1.2855	1.75091	-0.02363
15	-2.97795	-0.01118	-0.67959
24	1.101619	1.403382	-0.19221
24	-1.00358	-0.88144	-0.35916
7	2.137032	-1.84673	-1.19823
15	0.675337	-2.33328	-0.53991
15	2.287341	-0.18874	-1.36471
9	-1.29866	3.360186	-0.28096
9	-1.74132	1.89586	1.50423
9	-3.83931	-0.42061	-1.94035
9	-4.16828	-0.17184	0.353049
9	2.396738	-0.0205	-2.93717
9	3.857397	-0.10434	-1.11381
9	0.371465	-3.56251	-1.50017
9	1.175869	-3.24736	0.659961
6	3.232275	-2.77441	-1.49792
1	3.934633	-2.81957	-0.66501
1	2.822173	-3.76586	-1.67858
1	3.759502	-2.45075	-2.39378
6	-3.77113	2.666401	-1.07421
1	-4.63828	2.225613	-1.56426
1	-4.08668	3.120617	-0.13392
1	-3.35745	3.438615	-1.71917
6	0.857733	2.857845	0.962471
6	2.790117	2.194343	-0.1524
6	0.770183	2.298836	-1.8273
6	-2.00324	-2.42922	-0.43115
6	-0.80699	-0.67205	-2.21355
8	-0.70795	-0.54835	-3.35383
8	-2.64998	-3.38358	-0.47003
8	0.601644	2.840131	-2.823
8	0.842762	3.737424	1.700126
8	3.792911	2.74889	-0.10063
7	0.332373	-0.39604	2.707564
15	1.526686	0.255955	1.721821
15	-0.99419	-1.0389	1.88894
9	2.288416	1.087036	2.84041
9	2.60649	-0.92339	1.681456
9	-2.17343	-0.53545	2.818984
9	-0.9895	-2.50984	2.492203
6	0.550475	-0.65175	4.137379
1	-0.37833	-1.01001	4.575861
1	1.322061	-1.40831	4.285095
1	0.842371	0.266811	4.641999

Table S36: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ structure **35-3S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-2.36637	0.145991	1.793064
15	-1.76531	-1.32075	1.204916
15	-1.57549	1.591804	1.412011
24	0.376297	-1.43701	0.492271
24	0.01659	1.376939	-0.21207
7	3.175689	0.548643	0.210024
15	2.137736	1.881489	0.301977
15	2.523174	-0.98678	-0.06356
9	-2.17213	-2.24833	2.428954
9	-2.98855	-1.77441	0.287748
9	-1.37391	2.198984	2.860561
9	-2.82656	2.500867	1.06915
9	3.617892	-1.84366	0.707822
9	3.096306	-1.3029	-1.50801
9	2.693591	2.582954	1.608088
9	2.876393	2.864619	-0.69764
6	4.629434	0.761754	0.162403
1	4.968152	0.915655	-0.86285
1	4.881917	1.639385	0.754675
1	5.142985	-0.09711	0.587731
6	-3.67436	0.196893	2.463182
1	-3.67766	1.008263	3.189206
1	-4.47139	0.363585	1.737293
1	-3.85456	-0.73587	2.992109
6	0.610452	-3.26481	0.144965
6	0.884612	1.130379	-1.84601
6	0.843406	-2.13419	2.157639
6	0.652397	0.152664	1.655541
6	-0.22501	3.171393	-0.56796
8	0.949549	0.570632	2.708581
8	-0.36846	4.29252	-0.7934
8	1.11956	-2.58891	3.172726
8	0.808991	-4.38602	-0.00232
8	1.371199	1.055354	-2.89098
7	-1.59139	-0.59102	-2.32929
15	-0.46336	-1.62251	-1.64666
15	-1.68298	0.89458	-1.5525
9	-1.24916	-2.98893	-1.86928
9	0.537031	-1.85611	-2.85174
9	-3.23567	0.92641	-1.18511
9	-1.84891	1.834625	-2.82038
6	-2.38171	-0.93063	-3.51555
1	-3.28551	-0.32478	-3.52763
1	-1.81441	-0.73754	-4.42681
1	-2.66989	-1.97917	-3.48144

Table S37: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **34-1S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-0.40312	-1.03783	1.978167
15	-0.02961	0.003642	-1.7739
15	0.106418	0.458458	1.952011
24	-0.08963	-1.48283	-0.13395
24	0.060683	1.479567	-0.12856
7	3.075952	-0.1266	-0.05465
15	2.291345	1.352354	-0.20052
15	2.148413	-1.51565	0.10808
9	-1.21426	0.037627	-2.83043
9	1.118371	-0.04294	-2.86798
9	1.54953	0.538041	2.669071
9	-0.62847	1.24982	3.129396
9	2.760439	-2.11877	1.446209
9	2.964018	-2.47267	-0.86004
9	3.131255	2.208547	0.836587
9	3.041443	1.924786	-1.47782
6	4.543637	-0.20854	-0.08767
1	4.895619	-0.4091	-1.09938
1	4.968772	0.729673	0.261904
1	4.880434	-1.0042	0.574668
6	-0.36593	-1.93461	3.114009
1	0.60278	-2.43537	3.216003
1	-0.56269	-1.39838	4.045484
1	-1.13263	-2.70485	3.011367
6	0.018822	-2.35876	-1.74539
6	-0.19276	-3.28966	0.42253
6	0.00288	2.633557	-1.60204
6	0.205405	3.081762	0.869856
8	0.297975	4.063643	1.44862
8	-0.03795	3.348084	-2.4994
8	-0.25311	-4.39275	0.720233
8	0.083505	-2.9527	-2.73533
7	-3.09795	0.142412	0.062464
15	-2.34512	-1.3469	-0.08531
15	-2.15754	1.538969	0.024256
9	-3.09326	-2.14687	1.062526
9	-3.19049	-1.97496	-1.2709
9	-2.8127	2.32301	1.238131
9	-2.95731	2.341231	-1.0927
6	-4.5657	0.238853	0.092444
1	-4.86426	1.079834	0.715013
1	-4.96431	0.374546	-0.91273
1	-4.98024	-0.67029	0.522674

Table S38: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **34-2S** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	2.193608	0.139468	1.866415
15	1.778045	1.56531	1.117325
15	0.901542	-0.95235	1.704889
24	-0.23829	1.356282	0.199364
24	-0.2369	-1.35554	-0.19747
7	-3.31034	0.012642	0.022772
15	-2.31383	-1.20529	0.610763
15	-2.32256	1.215238	-0.60219
9	2.043641	2.642258	2.251507
9	3.109633	1.913734	0.316298
9	0.120765	-0.75087	3.075771
9	1.72252	-2.22188	2.216818
9	-3.25926	2.471529	-0.3342
9	-2.63025	1.153566	-2.15754
9	-2.61076	-1.16537	2.168569
9	-3.26815	-2.44598	0.32777
6	-4.77059	-0.02803	-0.00407
1	-5.13166	-0.61832	-0.847
1	-5.14194	-0.46973	0.919736
1	-5.1605	0.984774	-0.08222
6	-0.24601	3.106383	-0.40537
6	-1.05649	1.94878	1.81016
6	-1.06606	-1.94048	-1.80487
6	-0.25267	-3.10555	0.407172
8	-0.27912	-4.20583	0.747658
8	-1.58051	-2.30179	-2.76275
8	-1.56374	2.312303	2.770813
8	-0.26784	4.206912	-0.7453
7	2.186069	-0.14214	-1.87306
15	0.892947	0.948667	-1.70665
15	1.77694	-1.56939	-1.12354
9	1.712488	2.218133	-2.22146
9	0.108742	0.747345	-3.07569
9	3.111698	-1.91583	-0.32726
9	2.039478	-2.6458	-2.25858
6	3.37779	0.107471	-2.68456
1	3.100964	0.379281	-3.70303
1	3.96932	0.912092	-2.24852
1	3.980992	-0.79781	-2.71909
6	3.38824	-0.10808	2.67406
1	3.978694	-0.91308	2.237242
1	3.991021	0.797592	2.705017
1	3.115205	-0.37847	3.693941

Table S39: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **34-1T** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	-3.11934	0.200985	-0.37108
15	-2.15517	1.507422	0.038812
15	-2.26736	-1.17455	-0.84681
24	0.018406	1.297242	-0.52212
24	-0.06138	-1.37909	-0.3872
7	3.072627	-0.27154	-0.53184
15	2.127663	-1.47572	0.127499
15	2.111594	0.940813	-1.21422
9	-2.97806	2.685297	-0.64362
9	-2.67728	1.833705	1.506223
9	-2.79911	-1.35736	-2.33145
9	-3.24774	-2.26395	-0.22094
9	2.391254	0.725679	-2.76353
9	3.16949	2.126182	-1.05174
9	2.956114	-2.76471	-0.29654
9	2.647796	-1.4946	1.63627
6	4.5337	-0.23137	-0.47669
1	4.870459	0.471044	0.286744
1	4.912306	-1.22451	-0.24189
1	4.935805	0.070983	-1.44291
6	0.237834	3.146701	-0.90076
6	-0.56938	0.992728	-2.29833
6	-0.32864	-3.21364	-0.00022
6	0.396886	-1.72316	-2.21058
8	0.668253	-1.95544	-3.29924
8	-0.48378	-4.3262	0.224993
8	-0.89283	0.876775	-3.39654
8	0.361621	4.262483	-1.12682
7	0.225619	0.27791	2.637689
15	0.737868	1.497554	1.622239
15	-0.50287	-0.98417	1.778387
9	0.350271	2.780427	2.476242
9	2.291479	1.583204	1.978155
9	-2.01306	-0.85958	2.288838
9	-0.13509	-2.14466	2.812736
6	0.441675	0.258706	4.084432
1	1.295075	-0.37136	4.337943
1	0.626585	1.272677	4.434371
1	-0.44615	-0.12184	4.587898
6	-4.5758	0.204705	-0.21058
1	-4.8591	-0.23792	0.745301
1	-4.94188	1.228582	-0.2564
1	-5.03848	-0.36063	-1.01821

Table S40: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **34-2T** at M06-L/TZP level.

Atomic Number	M06-L		
	X	Y	Z
7	0.165051	1.006354	1.827527
15	0.025145	0.008567	-1.54527
15	-0.10525	-0.59469	1.858541
24	0.145545	1.773301	-0.06114
24	-0.1242	-1.70018	-0.13606
7	-3.00921	0.183592	-0.04491
15	-2.31026	-1.37226	-0.19337
15	-2.16865	1.627113	-0.00407
9	1.219982	0.014534	-2.62565
9	-1.12909	0.192103	-2.65431
9	-1.40367	-0.75749	2.78948
9	0.88701	-1.15796	2.979736
9	-2.83271	2.296175	1.272793
9	-2.98016	2.459463	-1.07905
9	-3.22702	-2.11493	0.871291
9	-3.14854	-1.85429	-1.45466
6	-4.48479	0.271491	-0.07959
1	-4.84344	0.293425	-1.1081
1	-4.90996	-0.58615	0.435572
1	-4.81165	1.172934	0.434126
6	0.230482	1.77328	3.064051
1	-0.65336	2.407584	3.177201
1	0.29419	1.126643	3.940786
1	1.110226	2.420484	3.06246
6	0.186134	2.738248	-1.73505
6	0.26252	3.537008	0.694818
6	-0.15259	-2.77188	-1.68591
6	-0.26614	-3.29965	0.880536
8	-0.35535	-4.287	1.455017
8	-0.17119	-3.41684	-2.63382
8	0.334808	4.624869	1.048155
8	0.212269	3.293068	-2.73228
7	3.010965	-0.23781	0.019891
15	2.411893	1.322636	-0.04623
15	2.085607	-1.67434	-0.08351
9	3.214285	1.974496	1.157802
9	3.311419	1.930519	-1.19795
9	2.843366	-2.48475	1.055766
9	2.888361	-2.34673	-1.28149
6	4.482607	-0.38469	-0.00653
1	4.764655	-1.2878	0.528689
1	4.844616	-0.44327	-1.03241
1	4.944798	0.464918	0.491097

Table S41: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_{10}$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-110-1S(C_1)**	**S-110-2S(C_1)**
B3LYP	E	-4399.734125	-4399.719331
	ΔE	0.0	9.3
	Nimg	0	0
BP86	E	-4400.189793	-4400.174150
	ΔE	0.0	9.8
	Nimg	0	0

Table S42: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginry vibrational frequencies (Nimg) for the three singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_9$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-19-1S(C_1)**	**S-19-2S(C_1)**	**S-19-3S(C_1)**
B3LYP	E	-4286.351553	Same to **S-19-1S**(B3LYP)	-4286.302976
	ΔE	0.0		30.5
	Nimg	0		0
BP86	E	-4286.800692	-4286.799201	-4286.761996
	ΔE	0.0	0.9	24.3
	Nimg	0	0	0

Table S43: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) and spin expectation values (S^2) for the two triplet stationary points of $MeN(PF_2)_2Cr_2(CO)_9$ using B3LYP/DZP and BP86/DZP methods.

Triplet		**S-19-1T(C_1)**	**S-19-2T(C_1)**
B3LYP	E	-4286.321098	-4286.312779
	ΔE	19.1	24.3
	$<S^2>$	2.05	2.04
	Nimg	0	0
BP86	E	-4286.764150	-4286.753660
	ΔE	22.9	29.5
	$<S^2>$	2.02	2.02
	Nimg	0	0

Table S44: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_8$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-18-1S(C_1)**	**S-18-2S(C_1)**	**S-18-3S(C_S/C_1)**
B3LYP	E	-4172.977360	-4172.975666	-4172.964777
	ΔE	0.0	1.1	7.9
	Nimg	0	0	0
BP86	E	-4173.429778	-4173.428848	-4173.423533
	ΔE	0.0	0.6	3.9
	Nimg	0	0	0

Table S45: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) and spin expectation values (S^2) for the two triplet stationary points of $MeN(PF_2)_2Cr_2(CO)_8$ using B3LYP/DZP and BP86/DZP methods.

Triplet		**S-18-1T(C_S)**	**S-18-2T(C_1)**
B3LYP	E	-4172.95933	-4172.955900
	ΔE	11.3	13.5
	$<S^2>$	2.10	2.09
	Nimg	0	0
BP86	E	-4173.407035	-4173.409428
	ΔE	14.3	12.6
	$<S^2>$	2.02	2.02
	Nimg	0	0

Table S46: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_8$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-28-1S(C_S)**	**S-28-2S(C_2)**
B3LYP	E	-5350.02306	-5349.961131
	ΔE	0.0	38.9
	Nimg	0	0
BP86	E	-5350.510816	-5350.462599
	ΔE	0.0	30.3
	Nimg	0	0

Table S47: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_7$ using B3LYP/DZP and BP86/DZP methods.

Singlet		S-27-1S(C_1/C_2)	S-27-2S(C_2)	S-27-3S(C_1)
B3LYP	E	-5236.664299	-5236.66366	-5236.625893
	ΔE	0.0	0.4	24.1
	Nimg	0	0	0
BP86	E	-5237.157236	Same to **S-27-2S**(BP86)	-5237.103175
	ΔE	0.0		33.9
	Nimg	0		0

Table S48: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) and spin expectation values (S^2) for the four triplet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_7$ using B3LYP/DZP and BP86/DZP methods.

Triplet		S-27-1T(C_1)	S-27-2T(C_1)	S-27-3T(C_2)	S-27-4T(C_1)
B3LYP	E	-5236.631905	-5236.630362	-5236.628066	-5236.624555
	ΔE	20.3	21.3	22.7	24.9
	$<S^2>$	2.05	2.04	2.06	2.04
	Nimg	0	0	0	0
BP86	E	-5237.101587	-5237.100114	-5237.100747	-5237.094019
	ΔE	34.9	35.8	35.4	39.7
	$<S^2>$	2.02	2.02	2.02	2.02
	Nimg	0	0	0	0

Table S49: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the four singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_6$ using B3LYP/DZP and BP86/DZP methods.

Singlet		S-26-1S(C_S)	S-26-2S(C_1)	S-26-3S(C_1)	S-26-4S(C_{2V})
B3LYP	E	-5123.305299	-5123.305149	-5123.263573	-5123.239976
	ΔE	0.0	0.1	26.2	41.0
	Nimg	0	0	0	0
BP86	E	-5123.787337	-5123.787972	-5123.756144	-5123.738088

ΔE	0.0	-0.4	19.6	30.9
Nimg	0	0	0	0

Table S50: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) and spin expectation values (S^2) for the one triplet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_6$ using B3LYP/DZP and BP86/DZP methods.

Triplet		**S-26-1T(C_S)**
B3LYP	E	-5123.285968
	ΔE	12.1
	$<S^2>$	2.06
	Nimg	0
BP86	E	-5123.770448
	ΔE	10.6
	$<S^2>$	2.02
	Nimg	0

Table S51: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_6$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-36-1S(C_1)**	**S-36-2S(C_1)**	**S-36-3S(C_1)**
B3LYP	E	-6300.341388	-6300.333324	-6300.293711
	ΔE	0.0	5.0	29.9
	Nimg	0	0	0
BP86	E	-6300.857522	-6300.864069	-6300.818777
	ΔE	0.0	-4.1	24.3
	Nimg	0	0	0

Table S52: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_5$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-35-1S(C_1)**	**S-35-2S(C_1)**	**S-35-3S(C_1)**
B3LYP	E	-6186.985596	-6186.977304	-6186.965454
	ΔE	0.0	5.2	12.6
	Nimg	0	0	0
BP86	E	-6187.508734	-6187.492193	-6187.491627
	ΔE	0.0	10.4	10.7
	Nimg	0	0	0

Table S53: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the two singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_4$ using B3LYP/DZP and BP86/DZP methods.

Singlet		**S-34-1S(C_1)**	**S-34-2S(C_1)**
B3LYP	E	-6073.624758	-6073.607875
	ΔE	0.0	10.6
	Nimg	0	0
BP86	E	-6074.142273	-6074.117842
	ΔE	0.0	15.3
	Nimg	0	0

Table S54: The energies (E, in kcal mol^{-1}), relative energies (ΔE, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) and spin expectation values (S^2) for the two triplet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_4$ using B3LYP/DZP and BP86/DZP methods.

Triplet		**S-34-1T(C_1)**	**S-34-2T(C_1)**
B3LYP	E	-6073.607184	-6073.605077
	ΔE	11.0	12.4
	$<S^2>$	2.09	2.08
	Nimg	0	0
BP86	E	-6074.117513	-6074.111244
	ΔE	15.5	19.5
	$<S^2>$	2.03	2.02
	Nimg	0	0

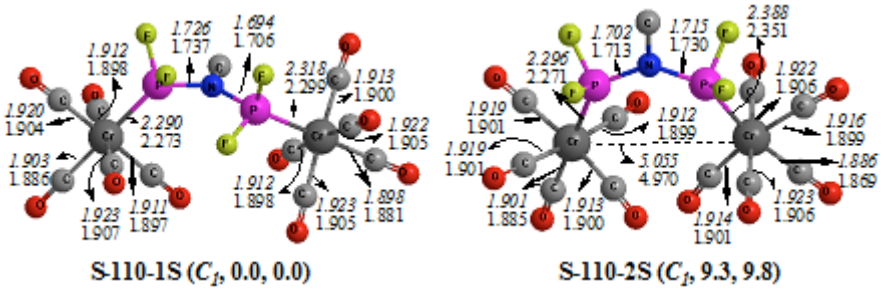


Figure S1: Optimized structures for $MeN(PF_2)_2Cr_2(CO)_{10}$ by B3LYP/DZP and

BP86/DZP methods. The upper distances were obtained by the B3LYP method and the lower distances by the BP86 method. All of the hydrogen atoms are omitted for clarity. The relative energies are shown in parentheses, predicted by the B3LYP method and the BP86 method, respectively.The data in all of the other figures in the present paper have the same arrangement.

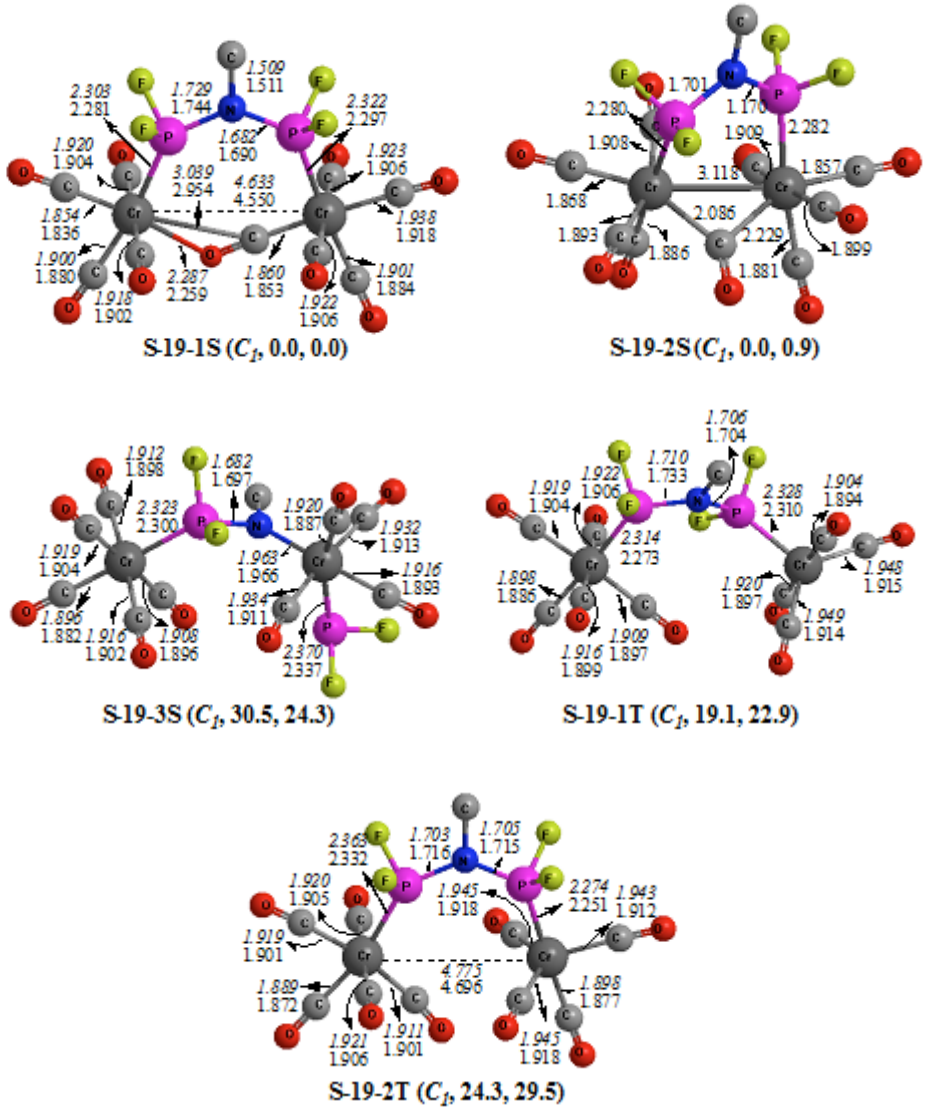


Figure S2: Optimized structures for $MeN(PF_2)_2Cr_2(CO)_{10}$ by B3LYP/DZP and BP86/DZP methods.

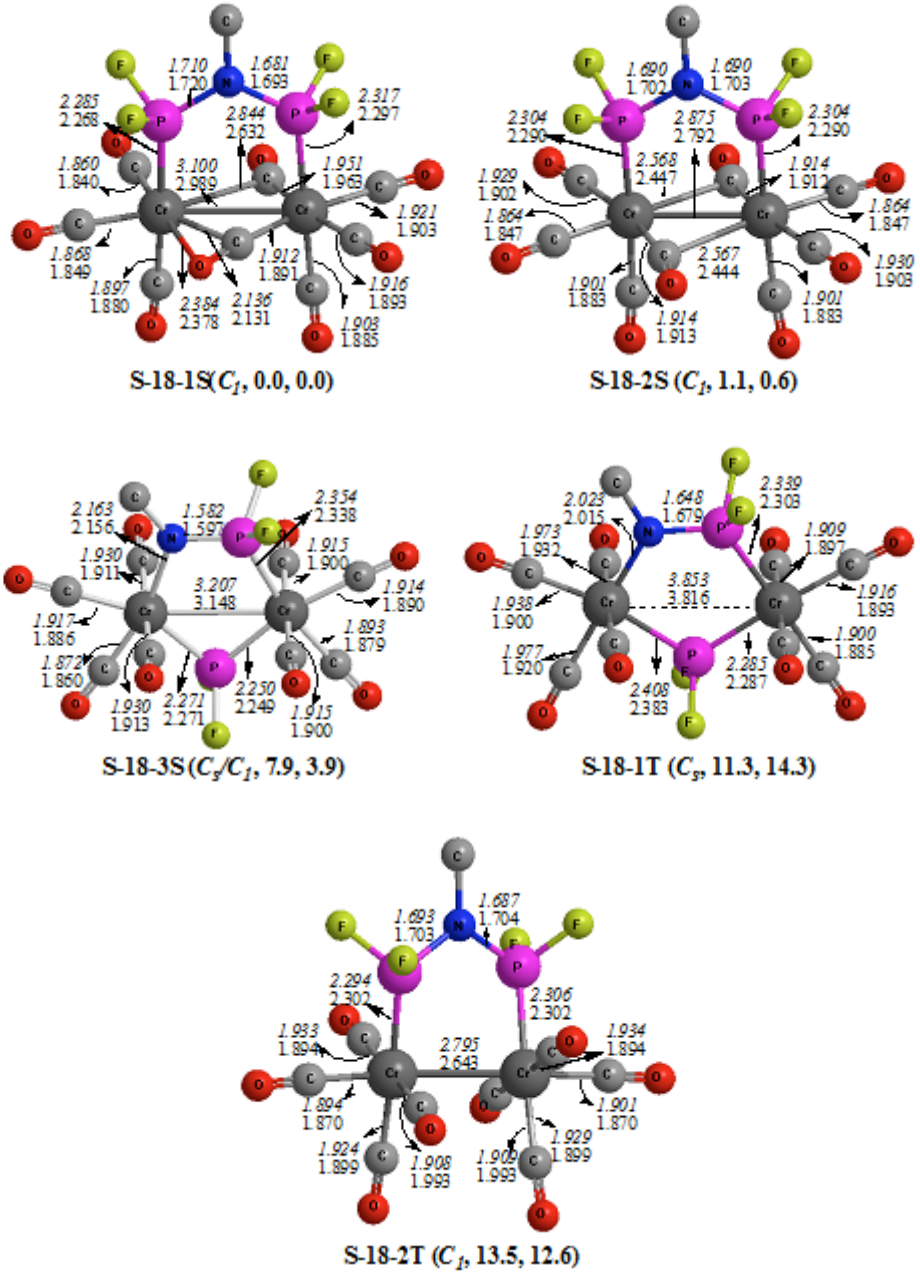


Figure S3: Optimized structures for $MeN(PF_2)_2Cr_2(CO)_8$ by B3LYP/DZP and BP86/DZP methods.

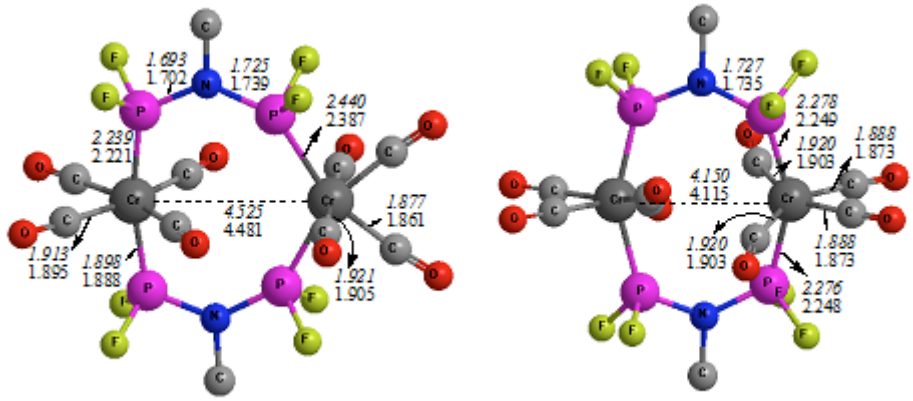
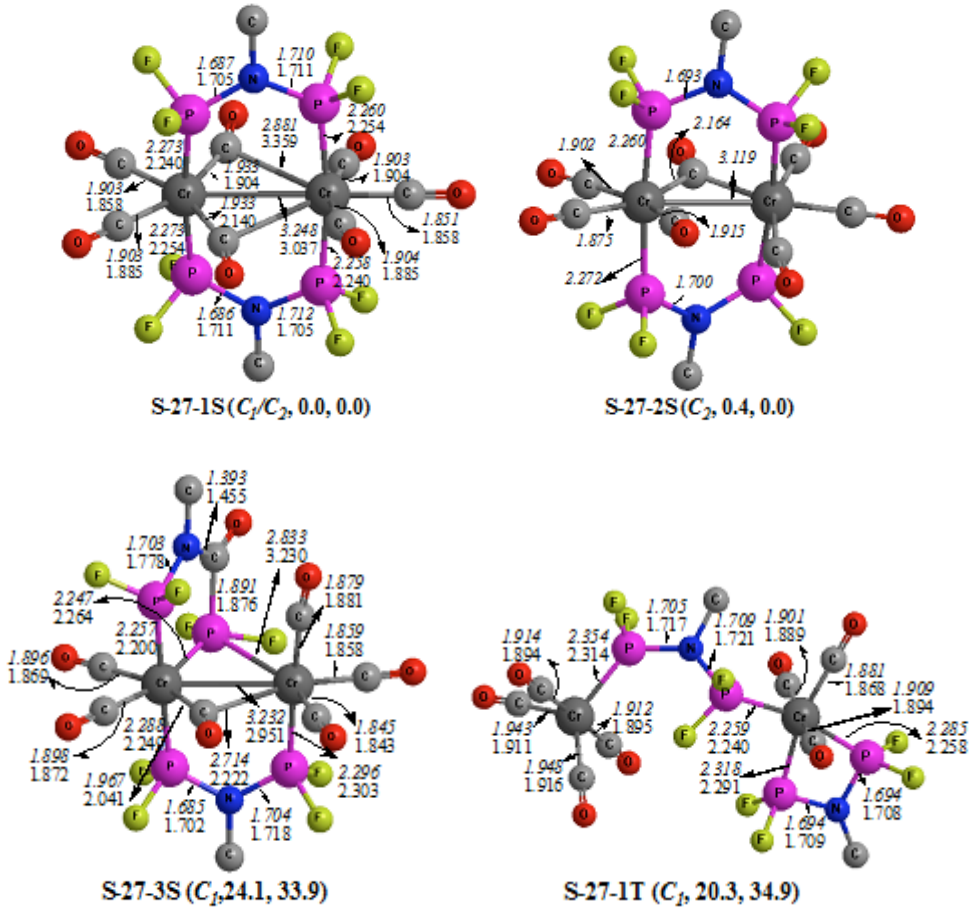


Figure S4: Optimized structures for $[MeN(PF_2)_2]_2Cr_2(CO)_8$ by B3LYP/DZP and BP86/DZP methods.



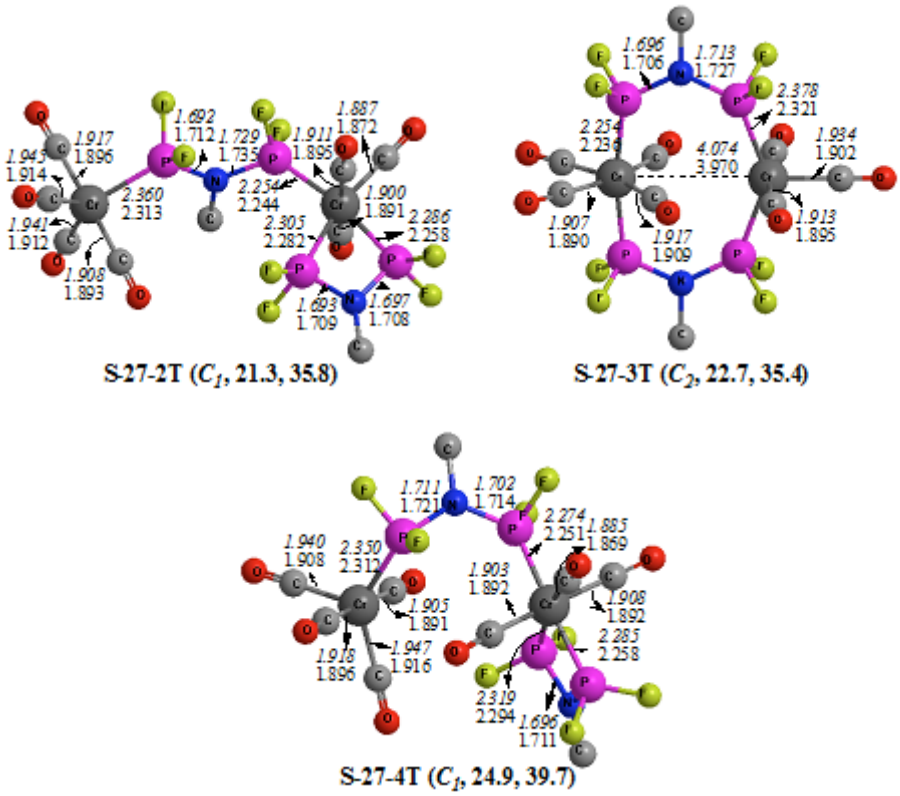
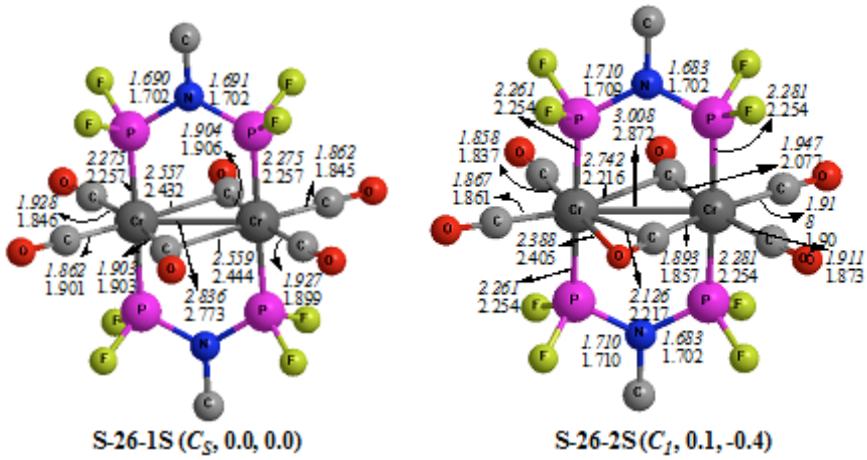
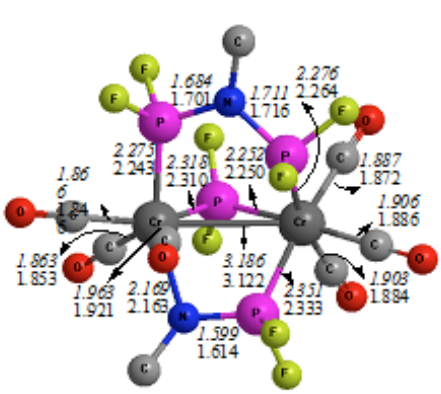
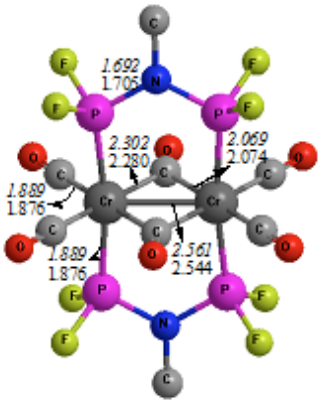


Figure S5: Optimized structures for $[MeN(PF_2)_2]_2Cr_2(CO)_7$ by B3LYP/DZP and BP86/DZP methods.

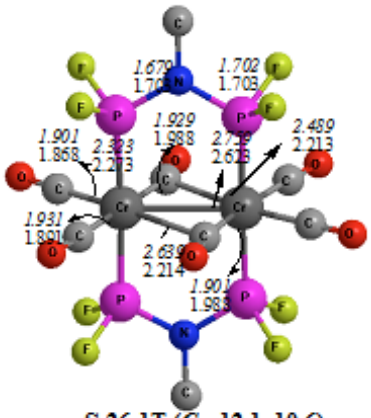




S-26-3S (C_1, 26.2, 19.6)

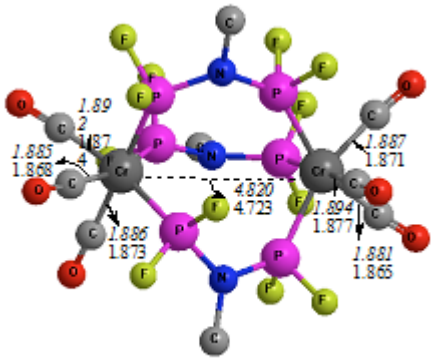


S-26-4S (C_1, 41.0, 30.9)

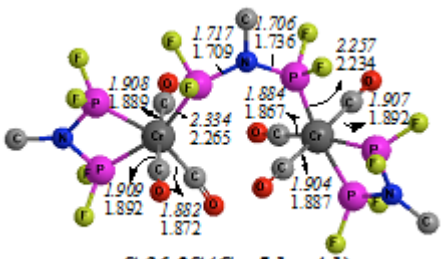


S-26-1T (C_S, 12.1, 10.6)

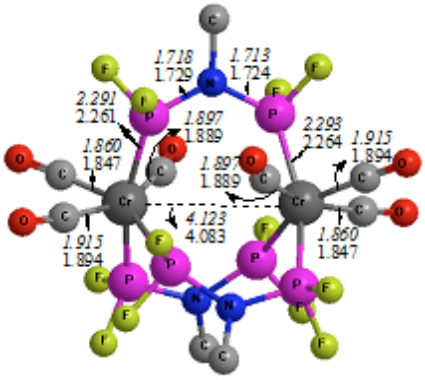
Figure S6: Optimized structures for $[MeN(PF_2)_2]_2Cr_2(CO)_6$ by B3LYP/DZP and BP86/DZP methods.



S-36-1S (C_1, 0.0 , 0.0)

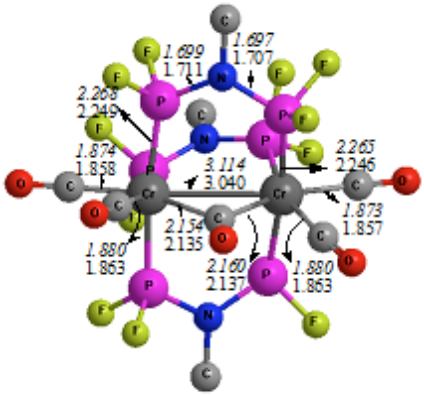


S-36-2S (C_1 , 5.1 , -4.1)

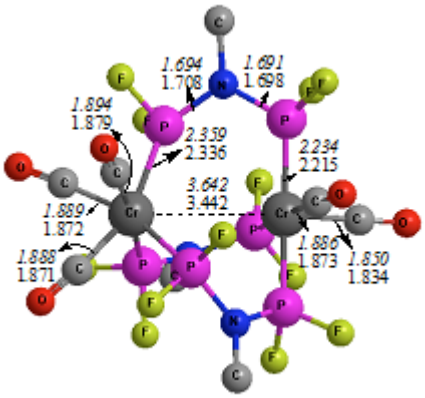


S-36-3S (C_1 , 29.9 , 24.3)

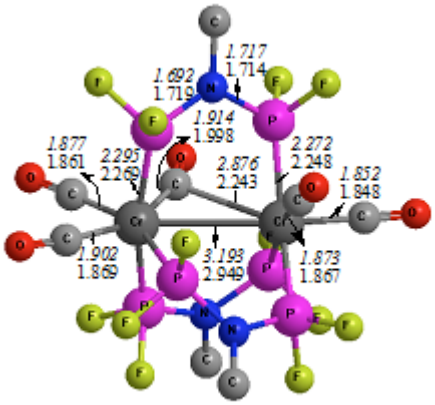
Figure S7: Optimized structures for $[MeN(PF_2)_2]_3Cr_2(CO)_6$ by B3LYP/DZP and BP86/DZP methods.



S-35-1S (C_1, 0.0 , 0.0)



S-35-2S (C_1 , 5.2 , 10.4)



S-35-3S (C_1, 12.6, 10.7)

Figure S8: Optimized structures for $[MeN(PF_2)_2]_3Cr_2(CO)_5$ by B3LYP/DZP and BP86/DZP methods.

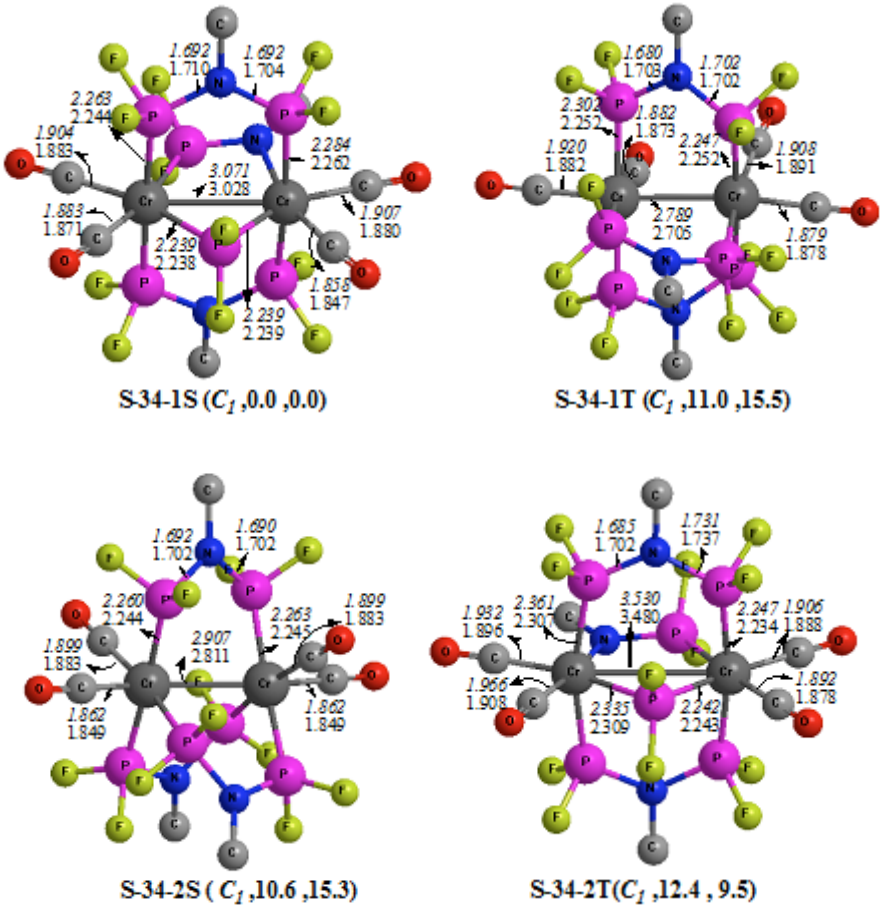


Figure S9: Optimized structures for $[MeN(PF_2)_2]_3Cr_2(CO)_4$ by B3LYP/DZP and BP86/DZP methods.

Table S55: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points of $MeN(PF_2)_2Cr_2(CO)_{10}$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	**BP86**
S-110-1S(C_1)	2035(1805),2043(60),2048(2500)	1959(1416),1965(48),1971(2302)
	2052(1892),2060(762),2063(729)	1973(1714),1982(663),1985(559)
	2074(346),2074(248),2139(465)	1994(207),1995(180),2058(492)
	2146(129)	2065(110)
S-110-2S(C_1)	2033(130),2036(2999),2051(982)	1955(101),1957(2557),1971(585)
	2055(49),2064(2878),2065(944)	1977(276),1983(2468),1986(672)
	2072(129),2073(10),2140(323)	1993(28),1993(149),2058(324)
	2148(224)	2066(223)

Table S56: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points and two triplet stationary points of $MeN(PF_2)_2Cr_2(CO)_9$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	BP86
S-19-1S(C_1)	1960(2120),2013(710),2029(934)	1876(1567),1939(655),1948(809)
	2049(677),2065(2259),2069(796)	1970(5850,1984(1890),1990(668)
	2085(354),2115(502),2147(297)	2002(3380,2032(546),2063(299)
S-19-2S(C_1)		1838(214),1948(237),1964(656)
	Same to **S-19-1S** (B3LYP)	1969(1057),1976(441),1982(1029)
		1987(809),2018(1435)
S-19-3S(C_1)	2032(1339),2036(10420,2050(1102)	1956(564),1957(895),1966(1106)
	2057(578),2062(678),2070(1189)	1971(1756),1978(570),1987(71)
	2099(444),2128(863),2141(293)	2000(497),2040(1029),2056(216
S-19-1T(C_1)	2005(1635),2037(2133),2046(59)	1936(1238),1954(340),1963(1088)
	2053(993),2058(1236),2059(1394)	1968(1110),1971(1635),1985(662)
	2072(220),2114(387),2144(237)	1994(171),2022(381),2062(265)
S-19-2T(C_1)	2030(175),2031(472),2038(2161)	1946(185),1950(416),1955(1574)
	2050(852),2055(687),2062(2440)	1963(628),1979(583),1980(1886)
	2071(93),2107(447),2143(273)	1991(140),2014(519),2060(298)

Table S57: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points and two triplet stationary points of $MeN(PF_2)_2Cr_2(CO)_8$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	BP86
S-18-1S(C_1)	1883(397),2007(107),2024(876)	1804(334),1916(95),1944(604)
	2037(1099),2067(1106),2074(1753)	1950(883),1987(476),1993(2034)
	2080(729),2133(720)	1998(615),2048(684)
S-18-2S(C_1)	1973(4),1998(1476),2031(982)	1885(8),1905(1006),1952(466)
	2037(161),2055(1093),2069(834)	1961(207),1974(1095),1981(550)
	2094(1740),2129(500)	2007(1768),2040(496)
S-18-3S(C_s /C_1)	2033(923),2047(154),2058(824)	1955(681),1960(44),1980(710)
	2087(527),2082(2434),2089(283)	1989(2164),1992(602),1997(194)
	2109(1920),2149(0.4)	2029(1495),2061(7)
S-18-1T(C_S)	2033(1112),2039(6819),2052(845)	1957(585,1963(1571),1973(592)
	2061(579),2080(1089),2104(1575)	1977(363),1992(1465),1994(1794)
	2146(155),2109(2330	2011(1311),2050(111)
S-18-2T(C_1)	1997(98),2003(3302),2022(3426)	1837(542),1842(6),1964(3),
	2049(78),2054(810),2057(2015)	1967(13),1969(1682),1982(632)
	2059(1160),2129(481)	1992(2549),2038(555)

Table S58: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_8$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	BP86
S-28-1S(C_S)	2007(227),2027(731),2029(2075)	1931(198),1949(1563),1954(565)

	2048(205),2057(2424),2068(210)	1972(350),1975(2011),1986(124)
	2114(783),2126(29)	2031(756),2043(69)
S-28-2S(C_2)	1981(258),2021(1951),2029(2838)	1905(206),1943(1416),1948(2211)
	2034(2),2038(6),2040(1194)	1954(0.4),1960(14),1961(177)
	2090(1194),2103(0.1)	2009(1246),2022(0.2)

Table S59: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points and four triplet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_7$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	**BP86**
S-27-1S(C_1/C_2)	1983(172),2001(162),2018(753)	
	2035(2081),2069(577),2078(1605)	Same to 27-2S(BP86)
	2112(241)	
S-27-2S(C_2)	1883(272),2015(238),2043(1253)	1798(216),1938(229),1965(381)
	2043(128),2053(2259),2080(1477)	1966(939),1973(1560),2000(1441)
	2111(2)	2028(2)
S-27-3S(C_1)	1790(272),1990(229),2001(261)	1715(294),1833(189),1942(574)
	2018(988),2057(2180),2063(645)	1952(504),1971(518),1989(2127)
	2098(587)	2013(479)
S-27-1T(C_1)	2009(1575),2024(1810),2030(761)	1934(1111),1947(1655),1952(64)
	2036(223),2050(1457),2089(304)	1953(648),1962(1216),2009(296)
	2110(309)	2020(239)
S-27-2T(C_1)	2009(1913),2022(1250),2035(699)	1933(1320),1948(730),1950(1059)
	,2044(660),2049(1251),2092(545)	1962(935),1966(631),2011(559)
	2110(319)	2020(272)
S-27-3T(C_2)	1989(147),2028(1399),2036(2756)	1916(94),1945(909),1955(2243)
	2041(0.3),2062(234),2088(1153)	1958(20),1979(160),2000(1172)
	2115(158)	2028(229)
S-27-4T(C_1)	2002(476),2020(2968),2038(272)	1927(357),1941(2398),1952(324)
	2041(765),2050(1040),2088(514)	1961(703),1964(592),2006(542)
	2111(270)	2020(192)

Table S60: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the four singlet stationary points and one triplet stationary points of $[MeN(PF_2)_2]_2Cr_2(CO)_6$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	**BP86**
S-26-1S(C_s)	1955(0.1)1980(1348),2036(74)	1869(0.3),1888(933),1958(1)
	2036(1849),2082(1819),2104(0.4)	1961(1408),1991(1800),2011(2)
S-26-2S(C_1)	1857(380),1988(33),2018(1197)	1788(333),1833(268),1952(597)
	2046(2190),2075(621),2108(613)	1974(2143),1981(405),2019(447)
S-26-3S(C_1)	2036(646),2046(745),2063(1488)	1948(428),1964(610),1972(1015)

	2066(798),2095(1749),2121(147)	1984(671),2007(1646),2027(226)
S-26-4S(C_{2v})	1799(759),1834(0.2),2047(1)	1761(511),1780(0.3),1961(0.3)
	2054(1922),2064(2361),2099(0.1)	1968(1625),1981(1807),2009(0.1)
S-26-1T(C_S)	1933(255),1958(538),2032(2510)	1820(517),1825(1),1960(0.3)
	2043(462),2063(2478),2099(6)	1961(1609),1981(2165),2007(0.1)

Table S61: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_6$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	**BP86**
S-36-1S(C_1)	2030(459) , 2036(1002), 2041(95),	1955(395), 1959(738), 1961(155),
	2043(1452), 2084(2545), 2096(48)	1964(1147), 2005(2247), 2016(60)
S-36-2S(C_1)	2007(181), 2022(1550), 2031(1226)	1937(1437), 1949(790), 1952(1001)
	2043(1464), 2085(292), 2094(124)	1966(511), 2006(522), 2012(98)
S-36-3S(C_1)	1991(150), 2002(1955), 2031(995)	1916(136), 1925(1601), 1954(405)
	2031(344), 2076(1726), 2087(83)	1954(395), 1995(1780), 2005(88)

Table S62: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the three singlet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_5$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	**BP86**
S-35-1S(C_1)	1871(251), 2030(1245), 2036(528)	1785(202), 1985(990), 1959(414)
	2061(1647), 2083(710)	1984(1470), 2002(568)
S-35-2S(C_1)	2006(895), 2044(645), 2046(281)	1930(686), 1965(287), 1967(429)
	2050(1902), 2095(1082)	1969(1632), 2015(952)
S-35-3S(C_1)	1973(413), 1997(843), 2034(1629)	1761(286), 1923(487), 1959(1576)
	2051(495), 2085(980)	1967(402), 1999(734)

Table S63: Infrared active (CO) vibrational frequencies (cm^{-1}) predicted for the two singlet stationary points and two triplet stationary points of $[MeN(PF_2)_2]_3Cr_2(CO)_4$ at B3LYP/DZP and BP86/DZP levels.(infrared intensities in parentheses are in km mol^{-1}).

	B3LYP	**BP86**
S-34-1S(C_1)	2021(1675),2017(121),	1942(588), 1974(583),
	2044(2324),2064(243)	1985(1841),2004(329)
S-34-1T(C_1)	1990(299),2020(2460),	1921(130), 1949(2180),
	2042(1827),2074(672)	1953(826), 1985(659)
S-34-2S(C_1)	2016(1675),2017(121),	1938(1168), 1939(125),
	2044(2324),2064(243)	1962(1995), 1980(196)
S-34-2T(C_1)	2043(760),2048(2962),	1949(913), 1963(637),
	2065(1070),2099(596)	1978(2273), 1998(312)

Table S64: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_{10}$ structure **S-110-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic	B3LYP			BP86		
Number	X	Y	Z	X	Y	Z
7	-0.019265	-1.063992	0.604176	-0.013153	-0.975348	0.63334
15	-1.658539	-1.304459	0.11967	-1.658573	-1.268119	0.161803
15	1.277638	-0.814393	-0.456945	1.300455	-0.799807	-0.440832
24	3.255653	0.279285	0.059166	3.274539	0.270162	0.054449
24	-3.167696	0.412634	-0.018538	-3.195485	0.394869	-0.030161
9	0.443704	-0.202571	-1.682284	0.48474	-0.239384	-1.718944
9	1.482716	-2.262537	-1.102216	1.493811	-2.299204	-1.005673
9	-1.43186	-2.195633	-1.17679	-1.417257	-2.206685	-1.116431
9	-2.034265	-2.480569	1.135507	-2.014563	-2.424736	1.230941
6	3.749843	-1.049411	1.343061	3.708774	-1.00932	1.389547
6	2.473807	1.384026	1.409476	2.527107	1.466759	1.324348
6	4.911756	1.149255	0.37749	4.937659	1.093088	0.360499
6	2.835165	1.637981	-1.234546	2.916393	1.570916	-1.291086
6	4.126378	-0.739824	-1.317682	4.138182	-0.808399	-1.25659
6	-1.761176	1.697531	0.127336	-1.842135	1.721782	0.055049
6	-3.402081	0.419194	1.879002	-3.428884	0.474903	1.852138
6	-4.598785	-0.857101	-0.183496	-4.581184	-0.906223	-0.138712
6	-2.995785	0.45414	-1.933746	-3.039557	0.373382	-1.93021
6	-4.436419	1.825265	-0.140139	-4.493592	1.752386	-0.199552
8	4.079723	-1.837965	2.123884	4.014491	-1.783843	2.21379
8	2.616667	2.470598	-2.003826	2.734268	2.385377	-2.109042
8	5.922476	1.676069	0.574145	5.975125	1.600314	0.552209
8	4.689421	-1.324202	-2.139306	4.713105	-1.4363	-2.057603
8	2.039924	2.080175	2.226014	2.121386	2.246025	2.099477
8	-5.208122	2.683132	-0.211463	-5.300733	2.593161	-0.302993
8	-5.480996	-1.596434	-0.284766	-5.456174	-1.67912	-0.209163
8	-2.917032	0.504901	-3.084252	-2.974207	0.389011	-3.096683
8	-3.561287	0.4477	3.025189	-3.598996	0.552912	3.008545
8	-0.906635	2.472997	0.213985	-1.015602	2.54967	0.103718
6	0.199422	-1.032343	2.077448	0.189428	-0.826337	2.10437
1	0.041279	-2.023959	2.510467	0.053712	-1.793503	2.615218
1	1.223154	-0.717174	2.282401	1.211874	-0.464086	2.289357
1	-0.475543	-0.310462	2.551931	-0.514062	-0.082033	2.518691

Table S65: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_{10}$ structure **S-110-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.233825	2.198211	-0.037558	-0.239491	2.197833	-0.036086
15	-1.795623	1.526729	0.038693	-1.812325	1.523462	0.030057
15	1.333221	1.502621	0.018258	1.342101	1.499148	0.027219
9	-2.363496	2.360425	1.28597	-2.399319	2.371677	1.278707
9	-2.475718	2.444776	-1.08506	-2.489497	2.440313	-1.118027
9	1.89346	2.362474	1.254216	1.893996	2.364708	1.283492
9	1.964575	2.423666	-1.1348	1.977974	2.440942	-1.128736
24	2.560028	-0.546353	-0.0037	2.51536	-0.53738	-0.006069
24	-2.494181	-0.660146	-0.007537	-2.453661	-0.655252	-0.005213
6	-0.225271	3.709308	-0.141704	-0.230281	3.71156	-0.138126
1	-0.248855	4.008839	-1.191748	-0.235485	4.016717	-1.195441
1	-1.092911	4.112292	0.383081	-1.114321	4.114343	0.377896
1	0.670516	4.10313	0.339411	0.663006	4.107095	0.366031
6	1.331329	-2.013053	-0.049081	1.296685	-1.995888	-0.049881
6	-1.319741	-1.128536	1.427802	-1.291545	-1.05761	1.442541
8	-0.686887	-1.419855	2.351401	-0.671677	-1.318102	2.401343
8	0.720952	-2.994719	-0.077184	0.692097	-2.997623	-0.076386
6	2.520611	-0.593473	1.917912	2.494331	-0.596293	1.899314
6	2.560621	-0.511485	-1.924971	2.517615	-0.496018	-1.911212
6	-1.320189	-1.051602	-1.465494	-1.299785	-0.992876	-1.475593
6	-3.075492	-2.469856	-0.049275	-2.940995	-2.47554	-0.039278
6	3.886108	-1.887438	-0.019382	3.816208	-1.879285	-0.035751
6	-3.8198	-0.283085	1.327993	-3.792577	-0.331287	1.305377
6	4.05757	0.648562	0.041794	4.02509	0.613666	0.041536
6	-3.826907	-0.229764	-1.319702	-3.806101	-0.289321	-1.290694
8	2.52551	-0.647026	3.071325	2.524044	-0.659997	3.065817
8	5.021558	1.285965	0.069399	5.016639	1.234482	0.071718
8	4.708465	-2.702008	-0.029014	4.643327	-2.708621	-0.054931
8	2.587072	-0.517039	-3.079556	2.558171	-0.49937	-3.07939
8	-4.641048	-0.085754	2.115671	-4.643084	-0.161629	2.08943
8	-4.652251	-0.002456	-2.09492	-4.664511	-0.095795	-2.060458
8	-0.68527	-1.286703	-2.403727	-0.682586	-1.204739	-2.448096
8	-3.412939	-3.574846	-0.074734	-3.227971	-3.609152	-0.06062

Table S66: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **S-19-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.088956	2.191194	-0.008451	-0.121945	2.196978	-0.00782
15	-1.611889	1.479682	0.038401	-1.649013	1.475459	0.05491
15	1.473526	1.451097	-0.008529	1.450192	1.443269	-0.022638
24	-2.290369	-0.741376	0.019281	-2.251893	-0.740584	0.013802
24	2.342644	-0.681674	0.029521	2.297674	-0.673515	0.034389
6	-0.091104	3.695613	-0.128266	-0.126888	3.703583	-0.126054
1	0.787817	4.09449	0.380238	0.766756	4.103149	0.375108
1	-0.080263	3.988007	-1.181052	-0.132707	4.00104	-1.186133
1	-0.978834	4.099574	0.362465	-1.013973	4.108194	0.384943
9	-2.323765	2.322145	-1.125285	-2.393064	2.330265	-1.100565
9	-2.270352	2.30164	1.247074	-2.306082	2.286625	1.291494
9	2.115372	2.362196	1.145235	2.109348	2.375648	1.126746
9	2.062607	2.302507	-1.233416	2.026595	2.292032	-1.275759
6	3.984201	0.16318	-0.140327	3.917726	0.174009	-0.127558
6	2.1857	-0.818809	-1.876652	2.178161	-0.816219	-1.858792
6	2.483872	-0.625817	1.943764	2.445588	-0.601793	1.931147
6	3.32439	-2.308144	0.038313	3.326799	-2.247022	0.052465
6	-2.133158	-0.78637	-1.895337	-2.09311	-0.753301	-1.885584
6	-4.104823	-0.080184	-0.143666	-4.073368	-0.160366	-0.136525
6	-2.457331	-0.724025	1.934495	-2.416796	-0.751977	1.912788
6	-3.009808	-2.500587	-0.013745	-2.908	-2.505451	-0.045153
8	5.039534	0.64331	-0.244473	4.98325	0.667758	-0.228881
8	2.613956	-0.607989	3.093608	2.597678	-0.569235	3.092434
8	2.13573	-0.916069	-3.029502	2.170121	-0.913368	-3.026949
8	3.965337	-3.271901	0.038822	4.028631	-3.185473	0.056878
8	-2.557075	-0.746547	3.084066	-2.518428	-0.794407	3.075724
8	-5.200678	0.263966	-0.239013	-5.197806	0.138799	-0.225409
8	-2.040075	-0.845902	-3.044424	-2.001744	-0.795912	-3.04963
8	-3.437097	-3.573931	-0.033212	-3.307704	-3.603909	-0.081872
6	-0.587801	-1.471993	0.178529	-0.548212	-1.45207	0.172609
8	0.467275	-1.967747	0.273261	0.49282	-2.010663	0.278558

Table S67: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **S-19-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15				-1.265882	1.620272	0.429061
15				1.488455	1.512003	-0.46076
24				1.528532	-0.689341	0.130226
24				-1.578201	-0.574873	-0.109821
6				0.150998	-1.315337	-1.305036
8				0.143598	-1.891024	-2.34389
6				1.003867	-0.153797	1.885294
6				2.613309	-1.079699	-1.37168
6				-1.940828	0.045217	-1.867353
6				-2.070869	-2.333281	-0.561618
6				1.45906	-2.494115	0.674729
6				-1.557974	-1.213514	1.689267
6				3.23079	-0.570675	0.88907
6				-3.397272	-0.316666	0.157216
8				0.889801	0.173837	3.004682
8	Same to **S-19-1S** (B3LYP)			4.301971	-0.534834	1.362145
8				1.435668	-3.610518	1.022721
8				3.339433	-1.325153	-2.253711
8				-1.701684	-1.642284	2.768519
8				-4.553733	-0.19184	0.313293
8				-2.251015	0.405154	-2.937378
8				-2.44411	-3.411489	-0.822163
9				-1.492436	2.131974	1.942368
9				-2.344694	2.626458	-0.23067
9				2.680144	2.431405	0.121773
9				1.700355	1.940354	-2.003149
7				0.155909	2.465757	-0.004458
6				0.179023	3.959411	-0.056146
1				-0.295806	4.322761	-0.982046
1				-0.356451	4.358998	0.820519
1				1.223989	4.303184	-0.010622

Table S68: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **S-19-3S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	0.487793	-0.777006	0.792512	-0.486463	0.666648	0.83544
15	-0.982852	-1.122311	0.052915	0.991921	1.09764	0.122017
24	-2.815858	0.304833	0.028922	2.824362	-0.287505	0.009099
24	2.220987	-0.407314	-0.05241	-2.231596	0.403821	-0.030865
9	-1.306248	-2.582393	0.650362	1.288535	2.523075	0.841992
9	-0.494909	-1.615536	-1.39127	0.495353	1.693909	-1.291656
6	0.332917	-0.780246	2.271828	-0.325116	0.453039	2.297873
1	0.831123	0.094095	2.705967	-0.736439	-0.536554	2.576793
1	-0.718336	-0.740123	2.58668	0.732416	0.480747	2.623708
1	0.761422	-1.692641	2.705101	-0.863036	1.236191	2.862861
6	3.129852	-0.933477	1.568676	-3.130589	0.850896	1.597483
6	3.966198	-0.007498	-0.735662	-3.966571	0.081366	-0.716262
6	1.479326	0.170969	-1.741851	-1.529462	-0.046289	-1.750634
6	2.521557	-2.112375	-0.88332	-2.526602	2.12334	-0.750349
6	-3.420687	-0.380135	1.708402	3.419689	0.289789	1.716677
6	-1.828239	1.672198	0.920495	1.891068	-1.732621	0.805415
6	-3.819071	-1.056674	-0.878605	3.791956	1.133447	-0.809368
6	-2.287556	1.024206	-1.666107	2.314968	-0.910602	-1.714315
6	-4.33903	1.432226	-0.014173	4.364587	-1.361729	-0.110211
15	2.564552	1.866765	0.520595	-2.583675	-1.862268	0.419123
9	2.830983	2.788215	-0.765786	-2.816338	-2.779305	-0.891383
9	3.991288	2.096671	1.224928	-4.003974	-2.171402	1.132726
8	2.662821	-3.139	-1.38138	-2.699315	3.180582	-1.211187
8	5.02543	0.223747	-1.138923	-5.047213	-0.101559	-1.133468
8	1.159933	0.538418	-2.785593	-1.237019	-0.330123	-2.845263
8	3.751887	-1.26747	2.480882	-3.77724	1.157423	2.523081
8	-4.447949	-1.857048	-1.426491	4.414897	1.983996	-1.316258
8	-3.810453	-0.771231	2.726131	3.817319	0.618755	2.768636
8	-1.234062	2.507914	1.460516	1.333946	-2.64046	1.296018
8	-5.270869	2.118912	-0.040078	5.32652	-2.026003	-0.184639
8	-2.004111	1.484842	-2.688371	2.046412	-1.323783	-2.775561

Table S69: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **S-19-1T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	0.275092	1.640213	-0.033051	-0.21785	-0.902771	0.405071
15	1.411063	0.665228	-0.851717	-1.527427	-0.622764	-0.648194
15	-1.425719	1.464723	0.004731	1.422933	-1.227512	-0.046626
24	3.169733	-0.434044	0.20664	-3.49474	0.306318	0.129138
24	-2.699979	-0.466133	0.060818	3.057764	0.348256	0.049651
6	0.845198	2.918812	0.507982	-0.426027	-0.753021	1.876393
1	0.777638	2.939223	1.597963	0.35015	-0.09495	2.306626
1	1.894376	3.003665	0.214424	-1.405673	-0.276351	2.052484
1	0.311731	3.773384	0.081559	-0.404005	-1.735551	2.376026
9	1.879025	1.651071	-2.022312	-1.742588	-2.033343	-1.396654
9	0.377457	-0.198943	-1.714147	-0.742099	0.088737	-1.866922
9	-1.862387	2.53755	-1.104312	1.165408	-1.940358	-1.4597
9	-1.678908	2.418855	1.264494	1.672468	-2.55289	0.840528
6	-2.517522	-0.739533	-1.833027	2.842042	0.725377	-1.806628
6	-4.247717	0.623688	-0.256052	4.348461	-0.984796	-0.379116
6	-1.214467	-1.612802	0.409924	1.806522	1.715411	0.454213
6	-3.845551	-1.977328	0.129821	4.443351	1.626738	0.101154
6	3.716599	1.11455	1.170114	-3.883343	-1.247016	1.140753
6	4.89291	-0.430036	-0.70223	-5.00904	-0.041722	-0.989684
6	2.726695	-2.060834	-0.712483	-3.164106	1.885093	-0.869128
6	2.727562	-1.310096	1.890815	-3.627428	1.387859	1.702509
8	-2.445523	-0.935456	-2.968702	2.742501	0.985334	-2.941406
8	-0.33152	-2.32361	0.645742	1.043252	2.568769	0.701451
8	-5.205718	1.243553	-0.439517	5.16682	-1.777779	-0.641993
8	-4.544519	-2.898077	0.17037	5.305806	2.416669	0.133565
8	2.486137	-3.054239	-1.256066	-2.989972	2.872384	-1.478099
8	5.92524	-0.437416	-1.220821	-5.952831	-0.234187	-1.654438
8	4.077913	2.040582	1.772648	-4.149667	-2.198193	1.777392
8	2.486307	-1.834025	2.891394	-3.744285	2.059813	2.655835
6	-2.940208	-0.253412	1.949913	3.348383	0.025724	1.898646
8	-3.105982	-0.158519	3.09008	3.551841	-0.146134	3.039038

Table S70: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_9$ structure **S-19-2T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.334826	2.223036	0.022924	-0.336703	2.229292	0.026803
15	-1.870176	1.482636	-0.016545	-1.877652	1.476906	-0.013128
15	1.220432	1.532234	-0.030765	1.230134	1.533184	-0.036192
24	-2.478048	-0.708137	0.003205	-2.439741	-0.702879	0.00169
24	2.294886	-0.57177	0.006338	2.254369	-0.560894	0.007751
6	-0.355414	3.72989	0.11906	-0.359818	3.738476	0.122603
1	0.520462	4.139618	-0.386502	0.514999	4.1518	-0.400856
1	-1.245197	4.10921	-0.386384	-1.26419	4.116179	-0.377441
1	-0.360422	4.037241	1.167443	-0.352198	4.050171	1.178337
9	-2.50511	2.31422	-1.234422	-2.526794	2.313661	-1.240737
9	-2.552656	2.354783	1.144708	-2.571428	2.348699	1.162995
9	1.878203	2.448961	1.110738	1.897081	2.465872	1.108743
9	1.7999	2.373364	-1.270144	1.804806	2.379223	-1.294435
6	3.89005	0.492924	-0.04613	3.854458	0.463168	-0.046195
6	2.246092	-0.627193	-1.913697	2.209	-0.623352	-1.896214
6	2.292619	-0.520789	1.92608	2.247054	-0.504197	1.911535
6	3.495515	-2.030353	0.033001	3.441682	-2.008137	0.042239
6	-1.695235	-1.024758	-1.748717	-1.666916	-1.006178	-1.726857
6	-4.343878	-0.16731	-0.027196	-4.286075	-0.208316	-0.027361
6	-1.723878	-0.967232	1.776887	-1.696495	-0.955562	1.751141
6	-3.05299	-2.517076	0.025994	-2.990021	-2.497253	0.021013
8	4.899796	1.053993	-0.076909	4.890515	1.005618	-0.078857
8	2.304111	-0.517769	3.081222	2.26385	-0.499238	3.080572
8	2.232395	-0.687271	-3.06697	2.20631	-0.690618	-3.063132
8	4.240859	-2.915383	0.049133	4.1987	-2.901439	0.063608
8	-1.308149	-1.143595	2.841824	-1.293604	-1.133602	2.83721
8	-5.467219	0.103949	-0.044555	-5.429482	0.045025	-0.04435
8	-1.265642	-1.239197	-2.801011	-1.249245	-1.219011	-2.800952
8	-3.403304	-3.621118	0.039549	-3.342372	-3.615863	0.032602
6	0.937983	-1.91609	0.060664	0.927061	-1.920257	0.063457
8	0.247498	-2.844438	0.094215	0.268758	-2.888555	0.098836

Table S71: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **S-18-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	-1.349124	1.638766	0.130884	-1.400355	1.613087	0.111691
15	1.571588	1.537999	-0.172455	1.522669	1.550917	-0.170498
24	-1.538772	-0.657815	-0.110404	-1.485577	-0.669558	-0.125581
24	1.559951	-0.746744	-0.160497	1.502933	-0.717331	-0.169654
6	3.308491	-0.768871	-0.817481	3.240094	-0.723601	-0.803912
6	2.229263	-0.717021	1.575092	2.230678	-0.689703	1.520245
6	-1.713951	-2.546625	-0.256661	-1.608607	-2.545167	-0.27393
6	1.646671	-2.639474	-0.061504	1.637912	-2.589873	-0.076842
6	-0.658219	-0.916308	1.611108	-0.483205	-0.877265	1.549553
6	-0.157861	-0.739501	-1.429801	-0.172311	-0.695102	-1.486244
6	-3.138605	-0.636555	0.952873	-2.986604	-0.741193	1.042519
6	-2.733164	-0.440395	-1.59246	-2.785565	-0.508028	-1.491541
8	-4.112938	-0.659962	1.569694	-3.919285	-0.82908	1.739206
8	-3.454114	-0.335283	-2.486848	-3.58719	-0.438983	-2.338636
8	0.594498	-0.815869	-2.339206	0.625526	-0.759472	-2.379424
8	-1.836141	-3.690943	-0.346478	-1.721276	-3.704215	-0.372544
8	1.777789	-3.786132	0.044804	1.828142	-3.74314	0.030485
8	-0.466987	-1.104608	2.738487	-0.339745	-1.044165	2.705729
8	2.677992	-0.734593	2.646852	2.738069	-0.707918	2.5812
8	4.392528	-0.81795	-1.230626	4.344965	-0.764455	-1.203529
9	2.145962	2.323802	-1.445897	2.099318	2.341556	-1.460533
9	2.503891	2.277083	0.891732	2.471509	2.295607	0.897528
9	-2.211341	2.545545	-0.864852	-2.270787	2.503133	-0.915816
9	-1.969796	2.259997	1.468297	-2.070996	2.229759	1.444923
7	0.132621	2.429684	0.070409	0.074731	2.444058	0.083691
6	0.188832	3.92073	0.160282	0.106921	3.9372	0.178958
1	0.950593	4.209631	0.889138	0.896385	4.236446	0.886684
1	0.425496	4.347134	-0.818994	0.299115	4.378772	-0.812619
1	-0.777937	4.302397	0.496545	-0.860809	4.298962	0.56019

Table S72: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **S-18-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.002826	2.485047	0.0219	0.000308	2.489879	-0.024075
15	1.443	1.611213	-0.028372	-1.446163	1.593204	-0.077551
15	-1.447472	1.60766	0.041812	1.445595	1.595423	0.068455
6	-0.009095	3.97639	-0.017497	-0.006153	3.983474	0.008989
1	-0.865395	4.34781	0.551725	0.928896	4.357845	-0.437161
1	0.904629	4.351253	0.450793	-0.8511	4.353546	-0.593793
1	-0.068096	4.330552	-1.050843	-0.098271	4.345973	1.045865
9	-2.265943	2.392675	-1.085878	2.153658	2.306442	1.333979
9	-2.188115	2.306795	1.274213	2.325548	2.363601	-1.044687
9	2.162394	2.322029	-1.266891	-2.302312	2.369571	1.048485
9	2.280289	2.386708	1.092042	-2.179104	2.296529	-1.333053
24	1.438452	-0.692459	-0.013155	-1.395201	-0.69338	0.029727
24	-1.436752	-0.69583	0.012166	1.396268	-0.692105	-0.028173
6	-0.492686	-0.781788	1.675162	0.380434	-0.710143	-1.649176
6	-2.929069	-0.726542	1.128017	2.790505	-0.691913	-1.239321
6	1.532085	-2.590115	0.053943	-1.493392	-2.573421	0.025311
6	-1.523572	-2.593224	-0.070444	1.49472	-2.571945	-0.009942
6	-2.694263	-0.670838	-1.45078	2.782531	-0.744092	1.273235
6	0.495794	-0.769686	-1.676972	-0.382487	-0.702481	1.651566
6	2.932226	-0.709315	-1.127384	-2.79414	-0.684975	1.235862
6	2.693982	-0.674588	1.451879	-2.776161	-0.755419	-1.277406
8	3.858166	-0.75491	-1.825397	-3.671728	-0.714966	2.016083
8	3.485578	-0.695453	2.290799	-3.668492	-0.835712	-2.028402
8	0.190069	-0.843346	-2.79914	-0.058461	-0.737609	2.787339
8	1.670525	-3.737782	0.081484	-1.661529	-3.732382	0.037046
8	-1.65769	-3.74113	-0.107565	1.662921	-3.730972	-0.012917
8	-3.486889	-0.687925	-2.28888	3.678016	-0.818716	2.021188
8	-3.854005	-0.780517	1.826715	3.66512	-0.726895	-2.022647
8	-0.187641	-0.862028	2.797017	0.059903	-0.750755	-2.785752

Table S73: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **S-18-3S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	1.916262	-0.60659	0	-0.611652	1.916876	-0.028169
24	-0.227521	-1.579073	0	-1.555047	-0.221918	0.025417
24	-0.08808	1.624873	0	1.5889	-0.066611	-0.003843
6	-0.181031	-1.599286	1.913852	-1.639734	-0.240956	-1.873038
6	0.675432	-3.266826	0	-3.235278	0.644259	0.007241
6	-1.778838	-2.663391	0	-2.629243	-1.758661	0.150965
6	-0.181031	-1.599286	-1.913852	-1.517475	-0.10143	1.920981
6	0.049804	1.615542	-1.924629	1.670595	-0.111293	1.904897
6	0.609035	3.410682	0	3.359159	0.582829	0.042497
6	0.049804	1.615542	1.924629	1.53414	0.231211	-1.892413
6	-1.675888	2.617135	0	2.57563	-1.625213	-0.244619
15	-1.750606	0.077585	0	0.080817	-1.764515	-0.016601
8	-0.15502	-1.665154	3.066247	-1.758891	-0.257979	-3.035716
8	1.183228	-4.301414	0	-4.295559	1.132252	-0.013063
8	-2.705612	-3.356343	0	-3.332737	-2.691254	0.236219
8	0.178613	1.663982	3.06833	1.580164	0.429886	-3.04184
8	-2.628366	3.281825	0	3.25568	-2.572768	-0.399756
8	-0.15502	-1.665154	-3.066247	-1.56228	-0.029681	3.087242
8	0.178613	1.663982	-3.06833	1.798448	-0.098148	3.064897
8	1.00092	4.493466	0	4.470626	0.939145	0.072061
9	2.868095	-1.170152	-1.179136	-1.333215	2.969452	0.981794
9	2.868095	-1.170152	1.179136	-0.994785	2.768644	-1.368128
9	-2.812134	0.142277	-1.188929	0.173293	-2.854098	1.162825
9	-2.812134	0.142277	1.188929	0.115346	-2.817196	-1.232154
7	1.974789	0.973875	0	0.959568	1.979473	0.249068
6	3.188673	1.794879	0	1.796208	3.186248	0.288015
1	3.22525	2.437094	0.890562	2.338481	3.341507	-0.664937
1	4.093669	1.174839	0	1.182879	4.084698	0.485227
1	3.22525	2.437094	-0.890562	2.538348	3.101968	1.103453

Table S74: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **S-18-1T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	1.017254	1.72974	-0.000019	-1.749814	0.999371	0
15	-0.62957	1.791687	0.000003	-1.790819	-0.67938	0
24	-1.891116	-0.177911	-0.000002	0.175715	-1.877044	0
24	1.959981	-0.060622	-0.000001	0.033907	1.93665	0
9	-0.978715	2.830038	1.183569	-2.836371	-1.017451	1.197117
9	-0.978744	2.830057	-1.183538	-2.836371	-1.017451	-1.197117
6	1.749193	3.016593	-0.000032	-3.044126	1.716	0
1	2.38475	3.092939	-0.891143	-3.114938	2.359715	-0.896225
1	1.070696	3.876648	-0.000058	-3.905274	1.025274	0
1	2.384726	3.092973	0.891094	-3.114938	2.359715	0.896225
6	-1.913536	-0.190338	-1.908469	0.188675	-1.908228	-1.89678
6	-3.544863	0.790015	-0.000012	-0.720575	-3.54487	0
6	-2.886998	-1.795819	-0.000008	1.804223	-2.827306	0
6	-1.91356	-0.190336	1.908465	0.188675	-1.908228	1.89678
6	1.889825	-0.083637	1.972013	0.0726	1.911641	1.931545
6	3.720764	0.747796	-0.000004	-0.721556	3.679786	0
6	1.889831	-0.083667	-1.972014	0.0726	1.911641	-1.931545
6	2.865469	-1.818378	0.000014	1.729399	2.837268	0
15	0.000419	-1.460161	0.00001	1.450914	0.020844	0
9	0.122687	-2.535311	-1.201975	2.533845	0.123323	-1.210188
9	0.122686	-2.535292	1.202012	2.533845	0.123323	1.210188
8	-1.95667	-0.212288	-3.065285	0.209513	-1.969464	-3.066346
8	-4.559486	1.343702	-0.000023	-1.231322	-4.598392	0
8	-3.497833	-2.779109	-0.000013	2.808461	-3.429309	0
8	1.842731	-0.05622	-3.118897	0.083054	1.926949	-3.096846
8	3.3826	-2.845208	0.000023	2.751831	3.400637	0
8	-1.956704	-0.21229	3.06528	0.209513	-1.969464	3.066346
8	1.842722	-0.056175	3.118895	0.083054	1.926949	3.096846
8	4.789587	1.182882	-0.000005	-1.104423	4.7865	0

Table S75: Atomic coordinates for the $MeN(PF_2)_2Cr_2(CO)_8$ structure **S-18-2T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	1.326817	1.53917	-0.498744	-1.454039	1.595742	-0.02894
15	-1.296084	1.532914	0.508864	1.451538	1.59853	0.018274
24	1.388435	-0.672594	0.14963	-1.320439	-0.70194	0.022361
24	-1.389575	-0.660977	-0.153714	1.321818	-0.699858	-0.021503
6	-3.211035	-0.725855	0.362299	2.64486	-0.705698	-1.34268
6	-1.778142	-0.066594	-1.951617	2.551674	-0.718188	1.418957
6	1.51943	-2.500493	0.753125	-1.542652	-2.58762	0.014334
6	-1.546195	-2.480876	-0.75914	1.548124	-2.584984	-0.001025
6	0.969944	-1.234772	-1.626523	-0.157667	-0.706271	1.640401
6	-0.997316	-1.24925	1.618588	0.158178	-0.716754	-1.63928
6	3.209655	-0.771869	-0.384539	-2.64423	-0.701191	1.342647
6	1.765554	-0.097781	1.957555	-2.550369	-0.73239	-1.418051
8	4.314912	-0.871857	-0.710691	-3.449401	-0.737729	2.193298
8	2.028595	0.22208	3.036251	-3.322942	-0.790198	-2.29485
8	-0.918739	-1.625863	2.715488	0.028209	-0.75008	-2.820828
8	1.641682	-3.592396	1.106692	-1.765972	-3.735633	0.010806
8	-1.684829	-3.571745	-1.112154	1.774013	-3.732445	0.01034
8	0.882693	-1.597246	-2.727526	-0.027243	-0.731557	2.822142
8	-2.053482	0.265985	-3.023638	3.324205	-0.768512	2.296318
8	-4.322756	-0.805039	0.674693	3.449556	-0.746646	-2.193531
9	-1.415037	1.9067	2.058096	2.28942	2.348836	-1.137034
9	-2.477218	2.498993	0.023619	2.212058	2.324726	1.239855
9	2.534895	2.472142	-0.018152	-2.241686	2.31104	-1.239648
9	1.438398	1.92378	-2.045409	-2.267075	2.354974	1.138239
7	0.023937	2.47477	0.022794	-0.001657	2.486225	-0.026493
6	-0.002809	3.962038	0.012357	-0.00534	3.980519	0.005232
1	1.023668	4.336366	-0.007891	-0.878218	4.349935	-0.556721
1	-0.548823	4.330758	-0.861256	-0.04549	4.344419	1.044783
1	-0.484514	4.320759	0.926894	0.906408	4.352823	-0.488683

Table S76: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_8$ structure **S-28-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	-0.002271	-1.909988	2.225643	-0.001364	-1.902026	2.20702
15	-0.007548	1.172526	2.127666	-0.006736	1.198735	2.101473
24	-0.008359	-2.157263	0	-0.009313	-2.149503	0
24	-0.000497	2.367326	0	-0.000837	2.331772	0
15	-0.007548	1.172526	-2.127666	-0.006736	1.198735	-2.101473
15	-0.002271	-1.909988	-2.225643	-0.001364	-1.902026	-2.20702
6	1.248482	-3.599488	0	1.221646	-3.590579	0
6	-1.278062	-3.588432	0	-1.257129	-3.576122	0
6	1.534347	-1.05105	0	1.537954	-1.067027	0
6	1.919991	2.406439	0	1.903485	2.374549	0
6	-1.546703	-1.043558	0	-1.550932	-1.057315	0
6	0.001465	3.803167	-1.208281	0.000399	3.771473	-1.17923
6	-1.922138	2.414998	0	-1.905967	2.383035	0
8	0.001895	4.758011	-1.866857	0.000229	4.751186	-1.826307
8	-3.06984	2.545432	0	-3.066443	2.525701	0
8	-2.576891	-0.509735	0	-2.604754	-0.538101	0
8	3.068621	2.531821	0	3.064999	2.511751	0
8	2.565395	-0.518709	0	2.592657	-0.549375	0
8	1.968537	-4.503049	0	1.937688	-4.515799	0
8	-2.006232	-4.485376	0	-1.984411	-4.492472	0
6	0.001465	3.803167	1.208281	0.000399	3.771473	1.17923
8	0.001895	4.758011	1.866857	0.000229	4.751186	1.826307
9	1.176832	-2.585577	3.071645	1.189041	-2.587441	3.059125
9	-1.194453	-2.570471	3.066496	-1.20615	-2.56826	3.055915
9	1.16556	1.826268	3.00543	1.177338	1.854428	2.993282
9	-1.224388	1.79234	2.971009	-1.237834	1.815969	2.957789
9	1.176832	-2.585577	-3.071645	1.189041	-2.587441	-3.059125
9	-1.194453	-2.570471	-3.066496	-1.20615	-2.56826	-3.055915
9	1.16556	1.826268	-3.00543	1.177338	1.854428	-2.993282
9	-1.224388	1.79234	-2.971009	-1.237834	1.815969	-2.957789
7	0.020369	-0.363003	2.912325	0.024788	-0.346652	2.89729
7	0.020369	-0.363003	-2.912325	0.024788	-0.346652	-2.89729
6	0.118932	-0.316837	-4.414556	0.124778	-0.297665	-4.40175
1	1.167332	-0.300941	-4.722957	1.180955	-0.284231	-4.713233
1	-0.380098	-1.193087	-4.833928	-0.382567	-1.178871	-4.823914
1	-0.39187	0.572855	-4.786255	-0.389168	0.600764	-4.773854
6	0.118932	-0.316837	4.414556	0.124778	-0.297665	4.40175
1	-0.380098	-1.193087	4.833928	-0.382567	-1.178871	4.823914
1	1.167332	-0.300941	4.722957	1.180955	-0.284231	4.713233
1	-0.39187	0.572855	4.786255	-0.389168	0.600764	4.773854

Table S77: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_8$ structure **S-28-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	2.87542	0.081613	-0.057917	0.059438	-2.869555	-0.049272
15	2.149043	1.612255	-0.360205	1.591874	-2.134304	-0.363837
15	2.212383	-1.456934	0.363304	-1.475901	-2.175661	0.364562
24	-0.047818	2.074225	0.012928	2.057302	0.032185	0.012629
24	0.047818	-2.074225	0.012928	-2.057301	-0.032185	0.012626
7	-2.87542	-0.081613	-0.057917	-0.059438	2.869554	-0.049286
15	-2.149043	-1.612255	-0.360205	-1.591873	2.134302	-0.363849
15	-2.212383	1.456934	0.363304	1.475901	2.175662	0.364554
9	3.184672	2.5275	0.450458	2.525673	-3.181181	0.44425
9	2.765756	1.900811	-1.806515	1.87907	-2.749696	-1.828241
9	2.828834	-1.61955	1.829169	-1.663599	-2.794485	1.843687
9	3.306775	-2.353225	-0.385094	-2.395863	-3.266329	-0.396361
9	-2.828834	1.61955	1.829169	1.663597	2.794493	1.843676
9	-3.306775	2.353225	-0.385094	2.395864	3.266327	-0.396373
9	-3.184672	-2.5275	0.450458	-2.525673	3.181183	0.444232
9	-2.765756	-1.900811	-1.806515	-1.879068	2.749688	-1.828256
6	-4.38052	-0.068194	-0.189149	-0.035863	4.37584	-0.174051
1	-4.670924	0.369804	-1.146902	0.395821	4.671456	-1.142773
1	-4.761899	-1.086499	-0.119618	-1.060228	4.763891	-0.087361
1	-4.813051	0.508656	0.632145	0.557728	4.801866	0.650237
6	4.38052	0.068194	-0.189149	0.035863	-4.375841	-0.17403
1	4.813051	-0.508656	0.632145	-0.55773	-4.801862	0.650259
1	4.670924	-0.369804	-1.146902	-0.39582	-4.671462	-1.142751
1	4.761899	1.086499	-0.119618	1.060227	-4.763892	-0.087336
6	-0.150094	3.570942	-1.133416	3.553563	0.067345	-1.114201
6	-0.50811	1.271965	-1.67011	1.2865	0.521302	-1.656903
6	-0.054607	3.547795	1.193396	3.525459	0.080109	1.175379
6	0.484399	1.274974	1.675381	1.283677	-0.512014	1.663357
6	-0.484399	-1.274974	1.675381	-1.283679	0.512022	1.663353
6	0.50811	-1.271965	-1.67011	-1.286497	-0.521309	-1.656902
6	0.054607	-3.547795	1.193396	-3.52546	-0.080101	1.175375
6	0.150094	-3.570942	-1.133416	-3.553561	-0.067353	-1.114205
8	0.08689	-4.506872	1.843446	-4.496765	-0.136405	1.831615
8	0.187239	-4.544744	-1.760964	-4.542612	-0.065087	-1.745921
8	0.923357	-1.064655	-2.733204	-1.069579	-0.944913	-2.731482
8	-0.923357	-1.073639	2.730003	-1.068809	0.95423	2.730752
8	-0.08689	4.506872	1.843446	4.496761	0.136414	1.831623
8	-0.187239	4.544744	-1.760964	4.542612	0.065078	-1.74592
8	-0.923357	1.064655	-2.733204	1.069583	0.944901	-2.731485
8	0.923357	1.073639	2.730003	1.068806	-0.954218	2.730758

Table S78: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-3.065485	-0.008589	-0.017412	3.052313	-0.412566	-0.057837
15	-2.258868	1.453913	-0.257444	2.438412	1.1445	-0.375763
15	-2.233291	-1.477979	0.253811	1.95894	-1.658003	0.36907
24	-0.006365	1.616852	-0.004577	0.256534	1.495928	-0.005935
24	0.006686	-1.630762	-0.00343	-0.256535	-1.495928	-0.005934
7	3.065297	0.024364	0.003476	-3.052315	0.412566	-0.057836
15	2.243669	-1.454168	-0.259342	-2.438412	-1.1445	-0.375763
15	2.248187	1.477983	0.252737	-1.958941	1.658003	0.36907
9	-2.888334	1.92146	-1.65224	3.490153	2.036718	0.465656
9	-3.168203	2.409286	0.647672	3.104208	1.448396	-1.813884
9	-3.129228	-2.436781	-0.663725	2.469148	-2.013816	1.86195
9	-2.923725	-1.915793	1.630282	2.724886	-2.892921	-0.339999
9	3.141822	2.4563	-0.64406	-2.469148	2.013815	1.861951
9	2.873742	1.941573	1.650508	-2.724887	2.89292	-0.339998
9	2.933051	-1.89374	-1.635824	-3.490155	-2.036719	0.465652
9	3.159045	-2.390242	0.662113	-3.104205	-1.448394	-1.813887
6	4.559992	0.000733	0.076683	-4.519765	0.693932	-0.12699
1	4.887721	-0.319446	1.069662	-4.786318	1.111746	-1.1114
1	4.944565	-0.687076	-0.681025	-5.073949	-0.241942	0.045819
1	4.948758	0.998597	-0.137814	-4.791492	1.407568	0.667437
6	-4.561642	-0.000331	0.027133	4.519764	-0.693933	-0.126991
1	-4.934819	-0.962772	-0.329225	4.791491	-1.407569	0.667435
1	-4.911972	0.181111	1.047286	4.786317	-1.111746	-1.111401
1	-4.939575	0.78057	-0.637819	5.073947	0.241942	0.045819
6	-0.122381	3.085403	1.199692	0.040989	2.478579	-1.600512
6	-0.24056	0.695835	1.678184	0.000005	-0.000006	-1.515549
6	0.094111	3.084863	-1.211089	0.529364	3.237589	0.580887
6	0.298367	-1.957314	1.848824	0.662072	1.166395	1.825229
6	-0.283954	-1.958614	-1.855977	-0.662072	-1.166385	1.825228
6	0.01733	-3.481668	-0.004958	-0.529366	-3.237586	0.580899
8	-0.454706	-2.326068	-2.94164	-0.040998	-2.478589	-1.600506
8	0.024313	-4.645083	-0.005936	-0.703441	-4.341098	0.942392
8	0.471239	-2.323788	2.934611	0.066468	-3.154998	-2.549038
8	0.150351	4.002156	-1.910562	-0.972856	-1.168833	2.956212
8	-0.188725	4.003083	1.897866	0.703442	4.341102	0.942378
8	-0.436613	0.544273	2.814733	-0.066475	3.154992	-2.549041
6	0.2387	0.697509	-1.686761	0.000011	-0.000006	-2.709801
8	0.436661	0.546572	-2.822908	0.972864	1.168845	2.95621

Table S79: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	3.04967	-0.412976	-0.044006			
15	2.462681	1.150619	-0.324099			
15	1.984159	-1.686286	0.320764			
24	0.258671	1.53798	-0.00837			
24	-0.258672	-1.537981	-0.008369			
7	-3.04967	0.412977	-0.044005			
15	-2.462683	-1.150619	-0.324098			
15	-1.984158	1.686287	0.320765			
9	3.489715	1.995072	0.565962			
9	3.169597	1.483222	-1.718904			
9	2.513949	-2.103747	1.773522			
9	2.74934	-2.860874	-0.452879			
9	-2.513947	2.103748	1.773522			
9	-2.749339	2.860875	-0.452879			
9	-3.489717	-1.99507	0.565962			
9	-3.169598	-1.483221	-1.718903			
6	-4.517665	0.68765	-0.103711			
1	-4.789741	1.093568	-1.082138			
1	-5.064737	-0.240393	0.077325	Same to **S-27-2S** (BP86)		
1	-4.78497	1.401003	0.680681			
6	4.517666	-0.687647	-0.103711			
1	4.78497	-1.401001	0.68068			
1	4.789742	-1.093564	-1.082139			
1	5.064736	0.240396	0.077326			
6	0.086519	2.499599	-1.640695			
6	0.000001	-0.000006	-1.508466			
6	0.534882	3.296509	0.580541			
6	0.603613	1.208064	1.846573			
6	-0.60361	-1.208058	1.846574			
6	-0.534883	-3.296509	0.580549			
6	-0.086523	-2.499607	-1.640691			
8	-0.707988	-4.386265	0.936644			
8	-0.005754	-3.151249	-2.591451			
8	-0.87362	-1.215015	2.973113			
8	0.707989	4.386267	0.936631			
8	0.00575	3.15124	-2.591457			
8	0.000003	-0.000004	-2.68588			
8	0.873621	1.215024	2.973113			

Table S80: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-3S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	2.766003	-1.311349	-0.3074	2.014697	1.903243	-0.239372
15	2.786209	0.390284	-0.22592	0.353076	2.200984	-0.559049
15	1.314383	-2.159843	-0.196485	2.495297	0.369324	0.321523
24	0.901373	1.628186	0.204934	-1.273027	0.87976	0.396737
24	-0.70144	-1.178418	0.258091	0.855149	-1.164095	0.441639
7	-3.204679	0.9465	-0.496667	-2.106355	-1.025251	-0.79481
15	-2.675305	-0.168165	0.677514	-1.116799	-2.111251	0.206591
9	4.038442	0.581059	0.744954	0.304232	3.72951	-0.024749
9	3.591825	0.70459	-1.575718	0.379554	2.656758	-2.109659
9	1.762736	-3.327431	0.801625	3.370786	0.767978	1.614949
9	1.396714	-3.056999	-1.518985	3.761019	0.086425	-0.63926
9	-2.915143	0.672816	2.007409	-2.167138	-2.404595	1.387912
9	-3.985052	-1.067578	0.821143	-1.352619	-3.520876	-0.548531
6	-4.445061	1.739404	-0.366297	-3.572371	-1.240527	-0.950066
1	-4.215308	2.724083	0.054275	-3.996341	-0.362622	-1.460524
1	-4.881104	1.8618	-1.361266	-3.753618	-2.1379	-1.567199
1	-5.146838	1.210641	0.283015	-4.029715	-1.361202	0.042245
6	4.04391	-2.065653	-0.490409	3.021142	2.990661	-0.442893
1	3.857533	-2.959511	-1.091423	4.005577	2.538037	-0.641646
1	4.756799	-1.434773	-1.026795	2.734393	3.590924	-1.321225
1	4.458817	-2.34995	0.480769	3.077602	3.635878	0.448807
6	1.769357	3.178415	-0.343385	-2.541804	1.89929	-0.4998
6	-2.383074	1.200471	-1.592671	-1.437235	-0.595459	-2.013082
6	1.515489	2.017318	1.901143	-1.228932	2.246873	1.632271
6	-0.573584	2.714601	0.622491	-2.586897	0.335472	1.628484
6	0.075786	-0.35302	1.86579	0.18264	0.109917	1.887866
6	-1.112575	-2.509841	1.547148	1.237648	-2.066239	2.036875
6	-1.52674	-2.453696	-0.877269	2.022726	-2.509395	-0.125416
8	-1.381178	-3.331221	2.313539	1.50509	-2.685071	2.994837
8	-2.037322	-3.270154	-1.518258	2.767917	-3.367604	-0.412453
8	0.330092	-0.278861	2.996278	0.341979	0.41536	3.026311
8	1.907965	2.331554	2.950756	-1.297846	3.070326	2.465921
8	2.284254	4.167479	-0.671594	-3.354264	2.55978	-1.033897
8	-2.63654	1.980887	-2.487214	-2.02339	-0.225294	-3.020531
8	-1.420542	3.450955	0.932066	-3.422311	0.174512	2.437256
15	-0.796604	0.173548	-1.534091	0.403578	-0.850386	-1.754458
9	-0.878307	-0.503962	-2.978755	0.623912	-2.154272	-2.690601
9	0.261823	1.326032	-2.008538	1.067654	0.181882	-2.788538

Table S81: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-1T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	4.260538	-0.152636	-0.332725	-4.263039	0.085843	-0.33054
15	2.17615	-1.61376	0.036674	-2.250697	1.613863	0.033955
24	2.194897	0.701361	0.14305	-2.189793	-0.673748	0.142906
24	-3.782695	-0.803866	0.050978	3.796729	0.775091	0.03607
15	-2.770384	1.233991	-0.550503	2.786182	-1.227428	-0.531694
15	0.024855	1.02184	0.682951	-0.028338	-0.925663	0.675276
6	2.681106	2.518266	0.154831	-2.633116	-2.487709	0.172345
6	1.772564	0.871576	-1.702994	-1.762119	-0.833057	-1.690151
6	2.569877	0.69782	2.014664	-2.558852	-0.675117	2.000333
6	-3.288969	-1.9728	1.5294	3.290611	2.087668	1.337206
6	-4.958892	0.119466	1.245567	4.785956	-0.088988	1.401048
6	-2.607054	-1.768933	-1.108286	2.795798	1.68892	-1.289053
6	-5.290889	-1.213847	-1.102622	5.408976	1.014844	-0.960982
8	-6.193854	-1.48634	-1.771851	6.405274	1.192345	-1.551719
8	-1.902208	-2.376414	-1.802303	2.192742	2.282281	-2.104374
8	-5.682918	0.655554	1.976241	5.413392	-0.595924	2.254595
8	2.805899	0.743342	3.147722	-2.79584	-0.723051	3.147656
8	2.992644	3.637294	0.157809	-2.933207	-3.62463	0.193815
8	1.506276	1.027904	-2.821311	-1.492864	-0.978015	-2.823969
8	-3.031413	-2.691938	2.396711	3.032143	2.917605	2.122231
9	-3.501195	2.588129	-0.098694	3.493675	-2.592635	-0.02442
9	-2.917346	1.508111	-2.122381	2.956499	-1.552476	-2.107965
9	-0.808067	-0.280361	1.116135	0.809211	0.420705	1.013389
9	-0.243208	1.855821	2.027435	0.27213	-1.678308	2.078341
9	1.465502	-2.509992	-1.069955	-1.550903	2.53291	-1.08337
9	1.940456	-2.627517	1.241617	-2.025489	2.635002	1.25473
9	5.054043	0.004413	-1.705896	-5.052236	-0.128419	-1.716063
9	5.553228	-0.09749	0.597619	-5.560155	-0.052014	0.611021
7	3.827426	-1.790272	-0.298707	-3.920611	1.758716	-0.297459
7	-1.143025	1.704579	-0.361098	1.133955	-1.662757	-0.358356
6	-0.761079	3.017238	-0.972026	0.740627	-2.997975	-0.917421
1	-1.016513	3.018931	-2.034175	1.093319	-3.081137	-1.956933
1	-1.267326	3.840949	-0.45963	1.154798	-3.817363	-0.306452
1	0.318451	3.155524	-0.87902	-0.358616	-3.069912	-0.920225
6	4.638576	-3.004104	-0.508884	-4.779201	2.943207	-0.507232
1	4.225105	-3.822218	0.089623	-4.417339	3.770522	0.126254
1	4.649235	-3.292314	-1.565518	-4.773256	3.256347	-1.565455
1	5.662435	-2.815767	-0.170212	-5.810212	2.699842	-0.200269

Table S82: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-2T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	4.279916	0.70694	-0.004416	4.525429	0.271096	-0.005042
15	1.841528	1.503452	-0.12967	2.354024	1.604538	-0.04942
24	2.481283	-0.702189	0.06601	2.474577	-0.670735	0.076057
24	-4.214629	0.552376	0.095302	-4.446061	0.527981	0.089095
15	-2.406286	-0.845501	-0.49402	-2.611742	-0.766705	-0.467773
15	0.476862	-1.733759	0.094907	0.355806	-1.409567	0.088831
6	3.419709	-2.335209	0.188549	3.078438	-2.440798	0.148965
6	2.471257	-0.681235	1.966017	2.457975	-0.676084	1.967255
6	2.527987	-0.943808	-1.829381	2.441022	-0.84503	-1.81052
6	-4.747575	0.993174	1.909077	-4.642409	1.49515	1.726795
6	-3.065679	2.075365	0.057944	-3.681201	2.044601	-0.746043
6	-5.392493	-0.958951	0.146011	-5.253919	-0.962612	0.937714
6	-5.175692	1.240746	-1.448819	-5.837392	0.488774	-1.224105
8	-5.766773	1.66686	-2.345609	-6.709958	0.482821	-2.00472
8	-6.124738	-1.856379	0.183093	-5.780536	-1.866996	1.468447
8	-2.381545	3.013895	0.043856	-3.228825	3.00247	-1.256189
8	2.577385	-1.139581	-2.969324	2.429926	-0.994773	-2.973249
8	4.006034	-3.33263	0.260755	3.475102	-3.544502	0.192626
8	2.477293	-0.716996	3.126426	2.448339	-0.720144	3.140533
8	-5.091784	1.274054	2.977981	-4.803407	2.093681	2.722627
9	-1.783786	-0.484665	-1.919714	-2.340831	-0.809365	-2.055626
9	-2.722926	-2.372579	-0.827855	-2.691319	-2.357679	-0.257413
9	0.006271	-2.490879	-1.22246	-0.085896	-2.320205	-1.159713
9	0.360361	-2.970384	1.10722	0.037698	-2.495078	1.243251
9	1.13472	2.199148	-1.376371	1.758844	2.47941	-1.266045
9	1.08926	2.377789	0.979098	1.866807	2.61565	1.114771
9	5.368979	0.817526	-1.162798	5.598391	0.104417	-1.191195
9	5.293235	1.007313	1.18867	5.607321	0.281724	1.185665
7	-1.013665	-0.939089	0.463155	-1.067414	-0.422927	0.187386
7	3.405026	2.152232	-0.158761	4.03447	1.901755	-0.136091
6	-1.065123	-0.353674	1.832719	-0.940403	0.834199	0.983279
1	-0.989376	-1.139751	2.591152	-0.199685	0.697815	1.788025
1	-0.262553	0.377499	1.970752	-0.648356	1.689057	0.348682
1	-2.018398	0.166399	1.964065	-1.909449	1.064114	1.459495
6	3.864823	3.548895	-0.271982	4.803297	3.160292	-0.227672
1	4.843502	3.565963	-0.762132	5.755699	2.963657	-0.747845
1	3.16039	4.112027	-0.892643	4.23028	3.891891	-0.821878
1	3.94163	4.019376	0.714214	5.008258	3.576054	0.774009

Table S83: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-3T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	2.243088	-0.003714	-1.644198	-0.093699	2.223905	-1.612074
15	2.239444	0.064655	1.412452	0.254513	2.188758	1.420413
24	0	0	-1.863049	0	0	-1.821725
24	0	0	2.21088	0	0	2.148404
15	-2.239444	-0.064655	1.412452	-0.254513	-2.188758	1.420413
15	-2.243088	0.003714	-1.644198	0.093699	-2.223905	-1.612074
6	-0.001677	-1.238759	-3.313076	1.208543	0.042697	-3.27361
6	-0.000132	-1.614051	-0.829308	1.627378	0.063436	-0.825829
6	0.001677	1.238759	-3.313076	-1.208543	-0.042697	-3.27361
6	0.000132	1.614051	-0.829308	-1.627378	-0.063436	-0.825829
6	-0.063958	1.907029	2.352775	-1.872141	0.25256	2.292333
6	0.063958	-1.907029	2.352775	1.872141	-0.25256	2.292333
6	0	0	4.144717	0	0	4.050586
8	0	0	5.301182	0	0	5.221885
8	0.10279	-3.049477	2.549883	3.017992	-0.410559	2.495475
8	-0.10279	3.049477	2.549883	-3.017992	0.410559	2.495475
8	0.002292	1.941604	-4.230909	-1.90087	-0.06827	-4.21731
8	-0.002292	-1.941604	-4.230909	1.90087	0.06827	-4.21731
8	0	-2.709548	-0.449813	2.748709	0.114895	-0.481959
8	0	2.709548	-0.449813	-2.748709	-0.114895	-0.481959
9	3.133062	-1.057676	2.131983	1.658989	2.886672	1.830802
9	3.050274	1.30254	2.035212	-0.658281	3.164508	2.339528
9	3.064536	-1.199367	-2.320536	0.995104	3.105752	-2.418538
9	3.060278	1.171883	-2.361276	-1.387945	2.981277	-2.214182
9	-3.050274	-1.30254	2.035212	0.658281	-3.164508	2.339528
9	-3.133062	1.057676	2.131983	-1.658989	-2.886672	1.830802
9	-3.064536	1.199367	-2.320536	-0.995104	-3.105752	-2.418538
9	-3.060278	-1.171883	-2.361276	1.387945	-2.981277	-2.214182
7	2.995992	0.012385	-0.124039	0	2.987164	-0.089575
7	-2.995992	-0.012385	-0.124039	0	-2.987164	-0.089575
6	-4.498041	0.06367	-0.117279	-0.074704	-4.490574	-0.091484
1	-4.823027	1.106448	-0.074266	-1.117225	-4.825826	-0.212804
1	-4.886829	-0.411407	-1.02049	0.543772	-4.877787	-0.916199
1	-4.883573	-0.482611	0.745946	0.337488	-4.870649	0.854902
6	4.498041	-0.06367	-0.117279	0.074704	4.490574	-0.091484
1	4.823027	-1.106448	-0.074266	1.117225	4.825826	-0.212804
1	4.886829	0.411407	-1.02049	-0.543772	4.877787	-0.916199
1	4.883573	0.482611	0.745946	-0.337488	4.870649	0.854902

Table S84: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ structure **S-27-4T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	0.239045	2.045386	-0.608078	0.250192	2.031717	-0.614932
15	-2.430787	1.153608	0.468959	-2.422734	1.136035	0.476241
24	1.72423	0.635787	0.381064	1.69495	0.616589	0.372966
24	-2.955011	-1.085902	-0.014398	-2.909032	-1.067953	-0.026971
15	1.803181	-1.031437	-1.228847	1.807419	-1.012126	-1.238358
15	3.332815	-0.919174	0.843454	3.285226	-0.914145	0.850201
6	1.993213	1.794739	1.84376	1.942661	1.751905	1.837209
6	0.530271	-0.303184	1.526784	0.512586	-0.321519	1.514121
6	3.031172	1.680801	-0.534614	3.010884	1.664076	-0.493072
6	-2.286061	-0.878066	-1.786427	-2.280407	-0.834225	-1.794809
6	-4.757125	-1.257733	-0.711335	-4.685642	-1.278296	-0.688804
6	-1.895997	-2.705497	0.201333	-1.886932	-2.677042	0.170695
6	-3.59432	-1.306683	1.780478	-3.534541	-1.308916	1.746654
8	-3.986782	-1.46644	2.858875	-3.935785	-1.488447	2.834731
8	-1.313626	-3.695154	0.330983	-1.325408	-3.696882	0.296136
8	-5.827082	-1.389614	-1.130059	-5.771304	-1.440368	-1.099228
8	3.843252	2.33918	-1.034583	3.845952	2.337123	-0.968802
8	2.165195	2.501169	2.746729	2.107187	2.457568	2.760577
8	-0.122634	-0.863147	2.30576	-0.122867	-0.889836	2.322125
8	-1.883956	-0.752881	-2.868931	-1.91525	-0.696221	-2.903559
9	-2.003117	1.545826	1.959574	-2.028347	1.532447	1.991662
9	-3.774062	2.016365	0.400461	-3.793605	1.986533	0.388494
9	0.631265	3.58885	-0.39471	0.663763	3.586551	-0.40063
9	0.346329	2.095283	-2.211237	0.343427	2.086952	-2.234482
9	3.349717	-1.947752	2.060546	3.279452	-1.946158	2.084175
9	4.908651	-0.682034	0.820411	4.869906	-0.638592	0.882855
9	2.294163	-0.860102	-2.734045	2.319463	-0.792722	-2.746928
9	0.721016	-2.160439	-1.547198	0.7228	-2.145804	-1.603239
7	-1.447333	2.211283	-0.449046	-1.44367	2.220168	-0.433067
7	3.055068	-1.91277	-0.499381	3.063759	-1.91823	-0.510878
6	3.717633	-3.160763	-0.922348	3.749185	-3.155884	-0.93824
1	4.582797	-2.950709	-1.560474	4.658547	-2.926177	-1.520021
1	4.042095	-3.714514	-0.035493	4.017918	-3.748331	-0.047496
1	3.000491	-3.780585	-1.469939	3.058138	-3.754419	-1.555061
6	-2.083176	3.403224	-1.105701	-2.07912	3.433708	-1.05477
1	-2.990318	3.098492	-1.632701	-2.980965	3.139719	-1.613753
1	-2.323472	4.170419	-0.364207	-2.338126	4.176743	-0.283133
1	-1.385083	3.81442	-1.836494	-1.363696	3.880233	-1.760978

Table S85: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **S-26-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	3.151538	-0.000464	-0.014732	-0.000644	0.019124	3.15498
15	2.274473	-1.445448	0.000704	1.444346	0.026298	2.255431
15	2.274847	1.444971	-0.003919	-1.44452	-0.029451	2.255832
24	0	-1.417876	0.00783	1.38603	-0.013231	0
24	0	1.418459	-0.016662	-1.386581	0.02146	0
7	-3.151539	-0.000464	-0.014733	-0.000644	0.019124	-3.15498
15	-2.274847	1.444971	-0.003912	-1.44452	-0.029451	-2.255832
15	-2.274473	-1.445447	0.000696	1.444346	0.026298	-2.255431
9	3.047917	-2.255661	-1.142763	2.23756	1.220169	3.002366
9	2.9941	-2.195732	1.217171	2.245058	-1.163561	2.999297
9	2.995982	2.21786	-1.204947	-2.280211	1.132354	3.004833
9	3.049009	2.231171	1.155848	-2.203461	-1.24991	2.995988
9	-3.047913	-2.255653	-1.142779	2.23756	1.220169	-3.002366
9	-2.994103	-2.195739	1.217157	2.245058	-1.163561	-2.999297
9	-2.995985	2.217869	-1.204932	-2.280211	1.132354	-3.004833
9	-3.049005	2.231164	1.155863	-2.203461	-1.24991	-2.995988
6	-4.641501	0.001643	0.032684	0.001066	-0.02392	-4.646914
1	-4.99108	0.022796	1.069187	0.031211	-1.066589	-5.003665
1	-5.017532	0.877222	-0.503176	-0.906651	0.47444	-5.023122
1	-5.017612	-0.895364	-0.466167	0.879859	0.525041	-5.021759
6	4.641499	0.001644	0.032684	0.001066	-0.02392	4.646914
1	5.01753	0.877216	-0.503185	-0.906651	0.47444	5.023122
1	4.991079	0.022807	1.069187	0.031211	-1.066589	5.003665
1	5.017611	-0.895369	-0.466158	0.879859	0.525041	5.021759
6	-0.000003	-2.923424	1.103473	2.80548	-1.193002	0
6	0.000001	-0.501508	1.675687	0.403008	-1.642523	0
6	0.000002	-2.67011	-1.458032	2.757685	1.302639	0
6	0.000002	2.675282	1.444682	-2.77833	-1.271085	0
6	0.000001	0.499263	-1.68381	-0.391277	1.647215	0
6	-0.000002	2.920576	-1.116836	-2.787993	1.221003	0
8	0.000001	0.202275	-2.813861	-0.084831	2.791586	0
8	-0.000003	3.855258	-1.806174	-3.670244	1.998435	0
8	0.000003	3.470536	2.281327	-3.681959	-2.01484	0
8	0.000003	-3.462708	-2.297042	3.649146	2.060459	0
8	-0.000004	-3.860283	1.789949	3.699701	-1.956709	0
8	0.000001	-0.202608	2.805335	0.084861	-2.783654	0

Table S86: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **S-26-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
15	2.259559	1.516823	-0.102759	2.254152	1.461382	-0.107975
15	2.281372	-1.426454	-0.01424	2.253583	-1.463441	-0.064127
15	-2.277982	-1.431058	-0.03016	-2.253667	-1.463474	-0.080409
15	-2.262523	1.512332	-0.12319	-2.252989	1.462791	-0.119465
24	0.001858	-1.472619	-0.069246	0.000099	-1.434506	-0.078931
24	-0.001293	1.534287	-0.138495	0.000773	1.437813	-0.10177
6	-0.001065	-3.036712	1.041683	-0.006497	-2.678705	1.364715
8	-0.002915	-3.991738	1.689271	-0.010811	-3.451427	2.239951
6	-0.010399	2.239875	1.580306	-0.003472	2.376674	1.477089
6	0.000067	3.289537	-0.775325	0.003919	3.154416	-0.820668
8	-0.016072	2.722671	2.638078	-0.006113	3.002862	2.471895
8	0.000737	4.38161	-1.173675	0.005798	4.246291	-1.255057
6	0.006275	-0.155552	-1.429175	0.005053	-0.264645	-1.521204
8	0.011234	0.6071	-2.339227	0.008285	0.59985	-2.356159
6	-0.005467	-0.548753	1.644655	-0.006124	-0.089328	1.504012
8	-0.010068	-0.379722	2.795661	-0.011673	-0.074699	2.693554
6	0.008609	-2.746847	-1.493011	0.005292	-2.958335	-1.16774
8	0.012729	-3.517596	-2.352244	0.008637	-3.903907	-1.860855
9	2.993681	-2.175356	1.207856	3.012852	-2.282449	1.102621
9	3.081513	-2.215001	-1.153624	3.005595	-2.216024	-1.281138
9	3.017269	2.325358	1.04803	3.015519	2.305476	1.035863
9	3.07325	2.187913	-1.310969	3.022091	2.170544	-1.344362
9	-3.062435	-2.239996	-1.166237	-2.99282	-2.235029	-1.293543
9	-3.002465	-2.162369	1.195307	-3.026803	-2.263331	1.090382
9	-3.061084	2.197225	-1.333783	-3.011223	2.197196	-1.347296
9	-3.039016	2.304088	1.026912	-3.024489	2.283345	1.034712
7	3.112342	0.037256	-0.006934	3.129945	-0.004682	-0.026651
7	-3.112708	0.030172	-0.050708	-3.12914	-0.004309	-0.076129
6	-4.603493	0.032188	0.040555	-4.622842	-0.010282	-0.031755
1	-4.920625	0.122292	1.083584	-4.975797	-0.002654	1.012426
1	-4.995317	0.871126	-0.540185	-5.001999	0.878419	-0.561121
1	-4.996526	-0.894132	-0.386307	-4.999577	-0.907876	-0.547817
6	4.606047	0.039288	-0.009577	4.62392	-0.012084	-0.061055
1	4.985818	0.103403	-1.033479	4.988462	-0.027681	-1.101339
1	4.962222	0.892802	0.572911	4.997816	0.887627	0.453058
1	4.972021	-0.875669	0.462993	4.993374	-0.898713	0.478561

Table S87: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **S-26-3S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	0.024695	2.432323	-0.658618	-0.054437	-2.417259	-0.671004
15	1.373884	1.639731	-0.988032	-1.409183	-1.603581	-0.999101
24	1.622661	-0.335716	0.262323	-1.581232	0.340472	0.279165
24	-1.31694	0.868919	0.020915	1.289333	-0.846321	-0.034002
7	-1.138461	-2.410462	-0.335788	1.132199	2.430373	-0.329853
15	-2.17282	-1.225072	0.266064	2.133415	1.20573	0.294347
15	0.404407	-1.893248	-0.865346	-0.406261	1.89732	-0.870763
9	1.553186	1.491743	-2.594155	-1.615483	-1.434601	-2.61422
9	2.584929	2.692674	-0.848529	-2.636078	-2.657902	-0.848212
9	0.19362	-1.817413	-2.452797	-0.215068	1.828481	-2.475227
9	1.093902	-3.33824	-0.889186	-1.124046	3.345786	-0.886195
9	-3.50143	-1.542152	-0.57033	3.520515	1.570467	-0.45301
9	-2.706612	-1.881907	1.61367	2.589249	1.817288	1.71272
6	-1.604485	-3.809341	-0.563506	1.600993	3.833829	-0.527546
1	-0.973969	-4.506547	-0.006061	0.972593	4.526176	0.054999
1	-2.635456	-3.901735	-0.213439	2.643373	3.911377	-0.180683
1	-1.572562	-4.049977	-1.630779	1.564166	4.101022	-1.596908
6	-0.354305	3.744701	-1.189398	0.334472	-3.725017	-1.215522
1	-0.945972	3.661732	-2.113224	0.921661	-3.630721	-2.150501
1	-0.954016	4.284434	-0.44641	0.949089	-4.264977	-0.472853
1	0.533907	4.351865	-1.406747	-0.56055	-4.339116	-1.427903
6	2.902108	0.647342	1.271906	-2.891975	-0.564031	1.285279
6	2.045597	-1.764086	1.420399	-1.860119	1.756177	1.471825
6	3.05272	-0.802214	-0.907745	-3.022114	0.855117	-0.823786
6	-1.673632	2.126798	1.347424	1.774191	-2.071205	1.268603
6	-3.092003	1.36826	-0.265906	3.045688	-1.302513	-0.374869
8	-4.19285	1.695943	-0.428279	4.161693	-1.612979	-0.579715
8	-1.938515	2.98488	2.079006	2.14384	-2.904709	2.010042
8	3.949601	-1.076533	-1.582504	-3.954241	1.155843	-1.464096
8	3.707403	1.186041	1.899445	-3.738398	-1.063239	1.9183
8	2.351563	-2.604361	2.157559	-2.082801	2.609402	2.246761
6	-1.390735	0.693097	-1.932686	1.35157	-0.680282	-1.947019
8	-1.511281	0.755134	-3.073435	1.483383	-0.733709	-3.104297
15	0.096138	0.331655	1.777617	-0.108852	-0.480572	1.76864
9	0.499064	1.480256	2.816129	-0.54722	-1.739819	2.676642
9	-0.467321	-0.678495	2.883861	0.44258	0.408523	2.994315

Table S88: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **S-26-4S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	3.159557	0	-0.017404	3.146781	0	0.020339
15	2.2956	-1.454141	-0.001955	2.272337	1.463187	0.0014
15	2.2956	1.454141	-0.001955	2.272337	-1.463187	0.0014
24	0	-1.280515	-0.003448	0	1.271769	0.003516
24	0	1.280515	-0.003448	0	-1.271769	0.003516
7	-3.159557	0	-0.017404	-3.146781	0	0.020339
15	-2.2956	1.454141	-0.001955	-2.272337	-1.463187	0.0014
15	-2.2956	-1.454141	-0.001955	-2.272337	1.463187	0.0014
9	3.031553	-2.251151	-1.171073	3.015566	2.273726	1.178247
9	3.035288	-2.226095	1.181604	3.019048	2.245226	-1.192388
9	3.031553	2.251151	-1.171073	3.015566	-2.273726	1.178247
9	3.035288	2.226095	1.181604	3.019048	-2.245226	-1.192388
9	-3.031553	-2.251151	-1.171073	-3.015566	2.273726	1.178247
9	-3.035288	-2.226095	1.181604	-3.019048	2.245226	-1.192388
9	-3.031553	2.251151	-1.171073	-3.015566	-2.273726	1.178247
9	-3.035288	2.226095	1.181604	-3.019048	-2.245226	-1.192388
6	-4.651544	0	0.026123	-4.641095	0	-0.021477
1	-5.003812	0	1.061645	-4.999329	0	-1.063694
1	-5.02457	0.88564	-0.495086	-5.014574	-0.892204	0.506299
1	-5.02457	-0.88564	-0.495086	-5.014574	0.892204	0.506299
6	4.651544	0	0.026123	4.641095	0	-0.021477
1	5.02457	0.88564	-0.495086	5.014574	-0.892204	0.506299
1	5.003812	0	1.061645	4.999329	0	-1.063694
1	5.02457	-0.88564	-0.495086	5.014574	0.892204	0.506299
6	0	-2.438328	1.489086	0	2.42026	-1.479503
6	0	-2.438138	-1.49668	0	2.419374	1.487683
6	0	2.438328	1.489086	0	-2.42026	-1.479503
6	0	2.438138	-1.49668	0	-2.419374	1.487683
8	0	3.127464	-2.425476	0	-3.121454	2.425921
8	0	3.127708	2.41794	0	-3.122837	-2.417477
8	0	-3.127464	-2.425476	0	3.121454	2.425921
8	0	-3.127708	2.41794	0	3.122837	-2.417477
6	0	0	-1.628321	0	0	1.642423
6	0	0	1.621261	0	0	-1.63532
8	0	0	-2.820471	0	0	2.845357
8	0	0	2.813589	0	0	-2.838407

Table S89: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ structure **S-26-1T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.0231	0.023192	3.168569	0.000133	-0.020975	3.161221
15	1.418779	0.001447	2.264038	-1.449888	-0.008962	2.268279
15	-1.471859	-0.013312	2.321126	1.45004	0.00683	2.268612
24	1.369703	-0.013067	0	-1.310989	0.009863	0
24	-1.388687	0.020018	0	1.311463	-0.017624	0
7	-0.0231	0.023192	-3.168569	0.000133	-0.020975	-3.161221
15	-1.471859	-0.013312	-2.321126	1.45004	0.00683	-2.268612
15	1.418779	0.001447	-2.264038	-1.449888	-0.008962	-2.268279
9	2.223482	1.154616	3.027553	-2.25993	-1.192967	3.006823
9	2.16373	-1.206208	3.007252	-2.242424	1.182952	3.014798
9	-2.288852	1.147951	3.056255	2.272428	-1.164873	3.014687
9	-2.238623	-1.207409	3.054743	2.23019	1.210568	3.007649
9	2.223482	1.154616	-3.027553	-2.25993	-1.192967	-3.006823
9	2.16373	-1.206208	-3.007252	-2.242424	1.182952	-3.014798
9	-2.288852	1.147951	-3.056255	2.272428	-1.164873	-3.014687
9	-2.238623	-1.207409	-3.054743	2.23019	1.210568	-3.007649
6	-0.001713	-0.018755	-4.659216	-0.000915	0.017712	-4.653878
1	0.060624	-1.052329	-5.012241	-0.023216	1.059255	-5.014036
1	-0.909425	0.451887	-5.04645	0.903091	-0.489599	-5.027279
1	0.860409	0.549577	-5.018005	-0.882727	-0.527757	-5.026834
6	-0.001713	-0.018755	4.659216	-0.000915	0.017712	4.653878
1	-0.909425	0.451887	5.04645	0.903091	-0.489599	5.027279
1	0.060624	-1.052329	5.012241	-0.023216	1.059255	5.014036
1	0.860409	0.549577	5.018005	-0.882727	-0.527757	5.026834
6	2.971773	-0.983391	0	-2.64271	1.319862	0
6	2.373707	1.626668	0	-2.53099	-1.435647	0
6	-2.31697	-1.673277	0	2.532883	1.426291	0
6	-2.898353	1.175035	0	2.641116	-1.330116	0
8	-3.784135	1.918722	0	3.450926	-2.178559	0
8	-2.906441	-2.666826	0	3.300396	2.310975	0
8	3.024277	2.58151	0	-3.297478	-2.321088	0
8	3.953929	-1.60112	0	-3.454112	2.166901	0
6	-0.43766	1.698718	0	0.163419	-1.640602	0
6	0.576991	-1.740483	0	-0.16431	1.633255	0
8	-0.239792	2.854519	0	0.044846	-2.826879	0
8	0.36173	-2.890493	0	-0.044867	2.819533	0

Table S90: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ structure **S-36-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic	B3LYP			BP86		
Number	X	Y	Z	X	Y	Z
24	2.362029	-0.09092	-0.3832	2.323402	-0.00334	-0.38189
24	-2.40154	0.322136	0.222952	-2.35294	0.296149	0.212602
7	0.032801	2.66985	-0.95254	0.013583	2.681267	-0.94672
15	-1.25822	1.606138	-1.28169	-1.24164	1.566846	-1.30822
15	1.518802	2.054426	-0.44937	1.399641	2.071344	-0.17828
9	1.725441	2.898474	0.900571	1.258733	2.691119	1.315247
9	2.465911	2.991465	-1.34342	2.43392	3.202696	-0.70037
9	-2.21549	2.707288	-1.93694	-2.2238	2.649863	-1.99581
9	-0.781	0.939023	-2.665	-0.72843	0.904017	-2.69815
7	0.485808	-0.16158	2.708558	0.502244	-0.37619	2.684324
15	-1.08442	-0.35243	2.045155	-1.10315	-0.40462	2.043929
15	1.957495	-0.25378	1.869614	1.96727	-0.44853	1.817473
9	2.58284	-1.55667	2.565107	2.538486	-1.87007	2.34252
9	2.786183	0.791247	2.754825	2.863353	0.445661	2.824314
9	-1.2852	-1.92373	2.332636	-1.4513	-1.95306	2.397223
9	-1.85036	0.163827	3.355213	-1.79107	0.22955	3.36541
6	0.580879	-0.29451	4.208702	0.607148	-0.60433	4.174277
1	0.174561	0.601975	4.680902	0.418966	0.340194	4.707089
1	0.032912	-1.17886	4.5449	-0.11836	-1.37039	4.489062
1	1.627173	-0.40614	4.494006	1.616812	-0.96763	4.414916
7	-0.62467	-2.28304	-1.52808	-0.56802	-2.26802	-1.54593
15	0.954735	-1.89906	-0.98022	1.043792	-1.80234	-1.13079
15	-2.07604	-1.57951	-1.02072	-2.03219	-1.60522	-0.99114
9	-2.83152	-2.87789	-0.46208	-2.72484	-2.93214	-0.37559
9	-2.83492	-1.56758	-2.43161	-2.85024	-1.65394	-2.38686
9	1.129241	-3.09303	0.084607	1.416013	-3.12723	-0.26576
9	1.702568	-2.63554	-2.19157	1.704848	-2.31808	-2.51583
6	-0.75172	-3.54767	-2.339	-0.68342	-3.52359	-2.37736
1	-0.35398	-3.38256	-3.34235	-0.51373	-3.28681	-3.43877
1	-0.21165	-4.36199	-1.84887	0.052076	-4.26582	-2.03067
1	-1.80394	-3.82508	-2.41037	-1.6884	-3.95171	-2.24861
6	-0.10833	4.144951	-1.17718	-0.1576	4.149665	-1.20498
1	-1.0425	4.499787	-0.73601	-1.11059	4.501339	-0.78026
1	0.722714	4.652872	-0.68394	0.669316	4.689036	-0.72076
1	-0.09022	4.375203	-2.2461	-0.13174	4.349398	-2.28846
6	-3.71871	-0.56165	1.253932	-3.69049	-0.52453	1.237069
6	3.578269	-1.53059	-0.28227	3.620872	-1.34612	-0.50066
8	-4.60127	-1.04678	1.825386	-4.60971	-0.97312	1.810975
8	4.416008	-2.32872	-0.22495	4.526641	-2.08853	-0.57166
6	-3.91	0.702928	-0.84085	-3.85674	0.659013	-0.83365
8	-4.8901	0.92426	-1.41731	-4.85995	0.866411	-1.40481
6	2.731055	0.094669	-2.23151	2.606545	0.447083	-2.18184
8	2.991424	0.214858	-3.35334	2.823124	0.740789	-3.29626
6	3.951203	0.843085	-0.01029	3.87944	0.920426	0.070123
8	4.981456	1.335705	0.189108	4.916255	1.412314	0.314652
6	-2.73625	1.921459	1.164679	-2.65373	1.908796	1.116039
8	-2.97146	2.912459	1.720895	-2.88001	2.927039	1.656057

Table S91: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ structure **S-36-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.08732	2.53637	0.021683	0.101924	1.154432	-0.39759
15	-1.66854	1.99822	0.370192	-1.5525	1.355111	-0.88415
15	1.379777	1.704859	-0.30356	1.203525	0.007352	-1.02372
9	-1.92764	2.929258	1.653125	-1.52236	2.944815	-1.19202
9	-2.46244	2.955748	-0.66043	-1.44283	0.847438	-2.40829
9	2.318513	2.762015	0.47954	1.381698	0.513825	-2.55043
9	1.651325	2.317933	-1.76592	0.154316	-1.17378	-1.37332
6	0.057686	4.042226	-0.00833	0.509488	2.056814	0.716153
1	0.4306	4.400756	0.953505	1.558047	1.849792	0.978003
1	0.747296	4.324791	-0.80581	0.427659	3.111259	0.404499
1	-0.9101	4.494756	-0.22329	-0.11133	1.878835	1.612065
7	5.416049	-0.76153	-0.05651	5.789083	0.637753	0.504805
15	4.506827	0.661129	-0.18486	4.330329	1.26782	-0.12318
15	4.132655	-1.85182	0.109727	5.212868	-0.95198	0.762474
9	5.152106	1.386042	-1.45085	4.811776	2.053046	-1.44416
9	5.173724	1.62	0.899713	4.080594	2.599622	0.760983
9	4.517803	-2.69836	1.405414	5.616001	-1.2649	2.290123
9	4.495038	-3.00481	-0.93124	6.362422	-1.87083	0.108454
7	-5.06218	-1.23103	-0.76824	-5.32033	-1.54969	-0.01829
15	-3.87071	-1.93135	0.215996	-5.0849	-0.39336	1.217427
15	-4.41958	0.332401	-0.88313	-3.99068	-1.08418	-0.98649
9	-4.44286	0.63173	-2.44863	-3.21845	-2.46534	-1.26712
9	-5.66415	1.263601	-0.52867	-4.63271	-0.95465	-2.45598
9	-3.48022	-3.26718	-0.55876	-5.1163	-1.25927	2.574721
9	-4.72335	-2.65722	1.351478	-6.55024	0.246234	1.4102
24	2.425926	-0.3674	-0.05918	3.124257	-0.66224	-0.02634
24	-2.57025	-0.06881	0.452066	-3.27559	0.636961	0.342361
6	6.874169	-0.97147	-0.04676	7.104665	1.260748	0.753509
1	7.34912	-0.24307	-0.71211	7.263552	2.072741	0.023977
1	7.281932	-0.86434	0.964419	7.166483	1.667445	1.77785
1	7.094479	-1.97518	-0.42418	7.895773	0.506054	0.607122
6	-6.28333	-1.80994	-1.35714	-6.32914	-2.61575	-0.18543
1	-7.04772	-1.03074	-1.44219	-6.50724	-2.78036	-1.26146
1	-6.08128	-2.23349	-2.34698	-5.99412	-3.55797	0.281812
1	-6.66546	-2.594	-0.69546	-7.27763	-2.29177	0.275213
6	-1.36544	-0.7865	1.709857	-3.06926	1.928477	1.675298
6	1.142846	-1.74041	0.042267	2.523236	-2.42144	0.193393
6	2.324223	-0.59281	-1.952	3.669232	-1.21661	-1.75155
6	2.326758	-0.13879	1.832467	2.459157	-0.386	1.719612
8	0.452597	-2.67304	0.070317	2.159037	-3.52783	0.334283
8	-0.70643	-1.21779	2.561512	-2.95035	2.739139	2.519191
8	2.249443	-0.00894	2.981589	2.045439	-0.29525	2.815625
8	2.233179	-0.75986	-3.09444	3.991164	-1.62821	-2.80192
6	-3.54141	0.484244	1.996644	-4.34342	1.904141	-0.57136
6	-1.56068	-0.54187	-1.09082	-2.08581	-0.46731	1.304204
8	-4.10294	0.808073	2.957098	-4.99015	2.724745	-1.10559
8	-0.97925	-0.79042	-2.06373	-1.31861	-1.10791	1.920533

Table S92: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ structure **S-36-3S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.73951	-2.16637	-1.73762	-0.61734	-2.15859	-1.72427
15	-2.21452	-1.68996	-1.03336	-2.12741	-1.68834	-1.07665
15	0.6927	-1.2105	-1.69306	0.803717	-1.15272	-1.66255
24	-2.05673	0.241484	0.104123	-2.03869	0.21954	0.070207
24	2.060496	0.224466	-0.11524	2.041224	0.210034	-0.07988
7	0.0118	3.092384	-0.01065	0.003153	3.07012	-0.01219
15	1.346909	2.305469	-0.75302	1.370185	2.275058	-0.71191
15	-1.34344	2.334013	0.712682	-1.37443	2.296331	0.678301
9	-3.17109	-1.70654	-2.31757	-3.05046	-1.70843	-2.40551
9	-2.70653	-3.10494	-0.47474	-2.64495	-3.11661	-0.52852
9	0.67444	-0.58143	-3.1648	0.768381	-0.50252	-3.14337
9	1.682662	-2.41765	-2.05861	1.814873	-2.35582	-2.06021
9	-2.44177	3.44476	0.352688	-2.47828	3.414497	0.283633
9	-1.17522	2.789103	2.235109	-1.25676	2.756303	2.220649
9	1.147149	2.731871	-2.27933	1.229338	2.709847	-2.25903
9	2.441055	3.4297	-0.42967	2.462883	3.410846	-0.3434
6	0.086506	4.592815	0.044269	0.069882	4.572693	0.039046
1	0.808229	4.910641	0.800981	0.770363	4.901037	0.822953
1	0.382775	4.977683	-0.93555	0.395967	4.957273	-0.94101
1	-0.89763	4.995472	0.283105	-0.93312	4.971558	0.245046
6	-0.74645	-3.35008	-2.6596	-0.58245	-3.34789	-2.64297
1	-0.37992	-3.05999	-3.64856	-0.22377	-3.05004	-3.6418
1	-0.12292	-4.14898	-2.25151	0.071143	-4.12923	-2.2259
1	-1.77135	-3.71169	-2.76436	-1.60363	-3.74639	-2.74433
6	-3.21526	-0.00939	1.607789	-3.26227	0.010033	1.50033
6	1.531029	0.900417	1.576103	1.483084	0.892027	1.590476
6	-3.68453	0.876728	-0.53306	-3.64549	0.810663	-0.62263
6	3.214485	-0.05841	-1.61709	3.262304	-0.02295	-1.50869
6	-1.52462	0.882264	-1.60064	-1.48106	0.874895	-1.61149
6	3.692	0.865167	0.506656	3.649427	0.812252	0.600617
8	-1.44534	1.35886	-2.6589	-1.39307	1.368755	-2.67726
8	4.737957	1.229902	0.853329	4.703324	1.158787	0.987352
8	4.035298	-0.13616	-2.43023	4.134118	-0.07139	-2.29249
8	-4.72863	1.237889	-0.88874	-4.69884	1.150069	-1.01704
8	-4.03826	-0.06918	2.420301	-4.13546	-0.02522	2.28335
8	1.449095	1.402827	2.622371	1.391025	1.406632	2.646257
7	0.726892	-2.13425	1.774455	0.613784	-2.1289	1.757502
15	-0.69896	-1.16863	1.70954	-0.80528	-1.1206	1.675498
15	2.205731	-1.68512	1.061469	2.125028	-1.67809	1.100373
9	-1.69678	-2.36259	2.096878	-1.81937	-2.31639	2.088186
9	-0.6774	-0.51346	3.169942	-0.77252	-0.44976	3.147324
9	2.686245	-3.11537	0.532477	2.635326	-3.11837	0.577227
9	3.162684	-1.68224	2.345509	3.05019	-1.67834	2.427953
6	0.723739	-3.30013	2.7189	0.573956	-3.30185	2.696702
1	1.746777	-3.66252	2.838285	1.595296	-3.69533	2.814801
1	0.351062	-2.98999	3.699399	0.205613	-2.98701	3.686731
1	0.100623	-4.105	2.321974	-0.07393	-4.09247	2.288233

Table S93: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ structure **S-35-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-2.74243	1.387998	-0.58739	-2.75719	1.35968	-0.60705
15	-1.35198	2.228373	-0.08935	-1.36584	2.188671	-0.05656
15	-2.66979	-0.28739	-0.84685	-2.63672	-0.32207	-0.87303
24	0.72626	1.379186	-0.41402	0.692771	1.354356	-0.40728
24	-0.72756	-1.37446	-0.42466	-0.69335	-1.35079	-0.41681
7	2.741221	-1.38101	-0.6031	2.757156	-1.3534	-0.61768
15	1.351306	-2.2248	-0.10838	1.365934	-2.18564	-0.07134
15	2.669211	0.296705	-0.84472	2.637369	0.330506	-0.86842
9	-1.65029	3.636868	-0.79029	-1.66665	3.63388	-0.71816
9	-1.80798	2.707501	1.375995	-1.83871	2.626449	1.433943
9	-3.30341	-0.3773	-2.31322	-3.24677	-0.42697	-2.36505
9	-4.00502	-0.73652	-0.09157	-3.98705	-0.81586	-0.13813
9	3.304423	0.402462	-2.30927	3.25079	0.449287	-2.35791
9	4.003422	0.738433	-0.08319	3.985805	0.818243	-0.12592
9	1.649909	-3.62887	-0.81784	1.668033	-3.6275	-0.73941
9	1.810391	-2.71175	1.353818	1.839774	-2.62936	1.417495
6	4.065608	-2.06795	-0.66833	4.088173	-2.02715	-0.70393
1	4.595032	-1.97311	0.284559	4.649795	-1.90221	0.236678
1	3.912816	-3.12276	-0.9054	3.93649	-3.09743	-0.91127
1	4.66118	-1.61809	-1.46746	4.656924	-1.58779	-1.53952
6	0.000702	0.012017	-1.91222	0.00245	0.007601	-1.91273
6	1.602966	2.966111	0.060163	1.561142	2.93542	0.036563
6	0.795187	2.329809	-2.03442	0.712539	2.323434	-1.99844
6	-1.60275	-2.96547	0.035743	-1.56008	-2.93512	0.017286
6	-0.79514	-2.30955	-2.05455	-0.7132	-2.3087	-2.01497
8	-0.87686	-2.945	-3.01822	-0.7642	-2.96923	-2.98153
8	-2.15097	-3.96635	0.2493	-2.11324	-3.95333	0.217624
8	0.877063	2.973839	-2.99236	0.763165	2.990532	-2.96052
8	-0.00069	0.014916	-3.09142	0.003823	0.010077	-3.10894
8	2.152176	3.96473	0.28097	2.115659	3.951751	0.242133
7	-0.01341	-0.0001	2.752988	-0.01613	0.003745	2.761318
15	0.984115	1.005111	1.842762	0.985916	1.007811	1.831984
15	-0.98588	-1.02194	1.832872	-0.98889	-1.02143	1.823235
9	0.890797	2.328617	2.738753	0.896284	2.348161	2.733206
9	2.430781	0.582061	2.393488	2.451122	0.588903	2.382375
9	-2.4396	-0.63221	2.389359	-2.46216	-0.63565	2.376312
9	-0.86276	-2.34625	2.724415	-0.87068	-2.361	2.722344
6	0.001118	-0.04021	4.239953	-0.00619	-0.03084	4.250379
1	0.699317	-0.80432	4.594689	0.695653	-0.79927	4.614168
1	0.294056	0.941024	4.621503	0.287268	0.960699	4.629853
1	-1.00626	-0.26587	4.600995	-1.02337	-0.2554	4.610514
6	-4.06702	2.075164	-0.64594	-4.08806	2.03412	-0.69021
1	-4.59942	1.964714	0.303578	-4.65325	1.897387	0.246582
1	-3.91407	3.133771	-0.86527	-3.9358	3.106952	-0.88346
1	-4.65977	1.638145	-1.45428	-4.65348	1.605277	-1.53351

Table S94: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ structure **S-35-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-0.7842	2.865444	-1.01154	-1.24849	2.743913	-0.99675
15	0.673395	2.304692	-0.35433	0.245971	2.362971	-0.26319
15	-2.09723	1.806371	-0.88944	-2.33971	1.447698	-0.88294
24	1.942255	0.317076	-0.29585	1.780734	0.603241	-0.33275
24	-1.64703	-0.29895	-0.29425	-1.47885	-0.50158	-0.27938
7	0.290263	-2.91678	-0.80125	0.738721	-2.87696	-0.7788
15	-1.15119	-2.46699	-0.03345	-0.74875	-2.58137	-0.00671
15	1.180919	-1.60953	-1.41597	1.408744	-1.44086	-1.41442
9	1.593874	3.422228	-1.04717	1.004402	3.678426	-0.84361
9	0.636038	2.998007	1.099092	0.047695	2.944323	1.241264
9	-2.81631	2.10183	-2.28673	-3.10787	1.596881	-2.29385
9	-3.12135	2.689325	-0.0322	-3.53767	2.105814	-0.01879
9	0.661821	-1.43745	-2.92296	0.93032	-1.39106	-2.95889
9	2.463866	-2.47701	-1.84468	2.845011	-2.10651	-1.79101
9	-2.16054	-3.52828	-0.67755	-1.64954	-3.7616	-0.64602
9	-1.02362	-3.2433	1.36179	-0.53958	-3.3384	1.406991
6	0.647348	-4.33878	-1.06706	1.301476	-4.23652	-1.01676
1	1.64682	-4.5532	-0.68061	2.327266	-4.29722	-0.62059
1	-0.07679	-4.97708	-0.55485	0.667387	-4.967	-0.48937
1	0.609358	-4.55196	-2.13988	1.298893	-4.47448	-2.09352
6	-0.9735	4.308351	-1.34203	-1.66016	4.137813	-1.33418
1	-2.01773	4.465311	-1.6226	-2.66847	4.097193	-1.77648
1	-0.74276	4.935342	-0.47497	-1.68696	4.771564	-0.43167
1	-0.33263	4.582821	-2.18331	-0.96257	4.561201	-2.07323
6	3.163312	1.568993	0.418985	2.807136	2.015956	0.340906
6	3.475209	-0.75752	-0.05206	3.495818	-0.12794	-0.17732
6	2.547947	0.801006	-2.02395	2.146978	1.198471	-2.07655
6	-3.44653	-0.64117	-0.03545	-3.18873	-1.12075	-0.04184
6	-1.98191	-0.73106	-2.0996	-1.72585	-0.96983	-2.07558
8	-2.31019	-0.995	-3.1809	-2.02119	-1.28516	-3.16864
8	-4.58216	-0.86324	0.098127	-4.29074	-1.52418	0.080703
8	2.970948	1.10079	-3.0586	2.431451	1.58628	-3.1453
8	3.992918	2.267444	0.82302	3.546845	2.836523	0.731754
8	4.471661	-1.31932	0.125898	4.609838	-0.4658	-0.0414
7	-0.01221	0.069554	2.752388	0.049035	0.034149	2.762884
15	1.386947	-0.28384	1.876928	1.454427	-0.11685	1.823482
15	-1.49446	0.153123	1.923478	-1.44104	-0.0538	1.925847
9	2.451067	0.265297	2.939046	2.486057	0.564088	2.867029
9	1.615541	-1.83392	2.230273	1.922698	-1.63767	2.137815
9	-2.0665	1.517034	2.538145	-2.19163	1.233545	2.554056
9	-2.3736	-0.79219	2.87286	-2.20959	-1.11711	2.874173
6	0.024479	0.113471	4.245442	0.11398	0.084408	4.254927
1	-0.9808	0.327034	4.614357	-0.91412	0.101834	4.648158
1	0.349074	-0.85189	4.646577	0.626414	-0.81056	4.645599
1	0.701248	0.904612	4.576753	0.641168	0.995489	4.579116

Table S95: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ structure **S-35-3S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-2.13829	0.80234	-1.88216	-2.36755	-0.10512	-1.84226
15	-1.31208	2.011119	-1.03263	-1.76051	1.384569	-1.23966
15	-1.68301	-0.85222	-1.76288	-1.5901	-1.57658	-1.43402
24	0.747215	1.498888	-0.18591	0.345929	1.458105	-0.42848
24	-0.36928	-1.4852	0.026926	0.018014	-1.40588	0.191781
7	3.002692	-1.11422	-0.20856	3.18569	-0.50607	-0.21877
15	1.695672	-2.12917	-0.66727	2.147195	-1.86231	-0.36537
15	2.716264	0.453719	0.358976	2.509041	1.038513	0.112414
9	-1.36107	3.185236	-2.11923	-2.07475	2.317103	-2.52374
9	-2.48333	2.613693	-0.11769	-3.03966	1.901072	-0.3868
9	-1.39684	-1.17879	-3.30306	-1.35764	-2.22637	-2.89007
9	-3.14738	-1.49552	-1.77165	-2.87698	-2.48762	-1.0941
9	4.024471	1.181544	-0.21312	3.595985	1.948348	-0.67039
9	3.246865	0.369045	1.862215	3.10918	1.339998	1.581367
9	2.152485	-2.53293	-2.14682	2.677807	-2.51905	-1.73797
9	2.215107	-3.49037	-0.00437	2.923204	-2.90965	0.586855
6	4.382941	-1.68332	-0.18667	4.665585	-0.7042	-0.23023
1	4.541797	-2.27218	0.721628	5.035105	-0.94848	0.779837
1	4.519131	-2.31895	-1.06625	4.909698	-1.52569	-0.92339
1	5.111487	-0.87137	-0.23452	5.152615	0.212469	-0.59663
6	-3.34909	1.149351	-2.68548	-3.63741	-0.14163	-2.62882
1	-3.34369	0.566704	-3.6111	-3.59708	-0.98603	-3.33596
1	-4.25904	0.93307	-2.11825	-4.50503	-0.25928	-1.95859
1	-3.31942	2.208886	-2.94841	-3.73285	0.789048	-3.20923
6	1.17636	3.086727	0.769075	0.502569	3.29636	-0.12947
6	0.360982	-2.01749	1.667092	0.907637	-1.24253	1.824995
6	1.574798	2.615722	-1.44689	0.891382	2.154498	-2.06611
6	0.883099	0.400642	-1.74696	0.605556	-0.15629	-1.57642
6	-0.96994	-3.22402	-0.18535	-0.19687	-3.22318	0.448195
8	1.14205	0.065298	-2.83422	0.898991	-0.50897	-2.68746
8	-1.33163	-4.32296	-0.31677	-0.31609	-4.38425	0.604876
8	2.080874	3.335756	-2.19786	1.228425	2.633876	-3.08025
8	1.523303	4.087877	1.233992	0.645584	4.45704	-0.02152
8	0.75401	-2.42901	2.683164	1.416659	-1.22969	2.888596
7	-1.7452	0.347666	2.324269	-1.56488	0.505963	2.429492
15	-0.28347	1.099622	1.923334	-0.47782	1.604438	1.714175
15	-2.09365	-0.98101	1.345356	-1.6674	-0.97663	1.611631
9	-0.66351	2.515761	2.58998	-1.33863	2.952949	1.976338
9	0.694274	0.655422	3.106019	0.551278	1.866912	2.929105
9	-3.5984	-0.64045	0.90317	-3.2514	-1.0367	1.274206
9	-2.53445	-2.05699	2.443776	-1.77319	-1.98324	2.872089
6	-2.57367	0.764146	3.486865	-2.3695	0.852594	3.633734
1	-3.36643	0.025087	3.62832	-2.75017	-0.0775	4.08445
1	-1.96144	0.796351	4.393417	-1.72334	1.357379	4.370963
1	-3.01888	1.745631	3.303156	-3.21162	1.509444	3.360955

Table S96: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **S-34-1S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	0.203819	1.058458	1.928791	0.243941	1.065668	1.939955
15	0.006262	-0.00137	-1.79972	0.004967	0.000508	-1.79944
15	-0.05483	-0.50338	1.954588	-0.05325	-0.50486	1.960845
24	0.064117	1.54844	-0.18446	0.063174	1.525133	-0.16018
24	-0.05297	-1.52027	-0.15615	-0.05328	-1.501	-0.14094
7	-3.09826	0.103113	0.010277	-3.09997	0.104512	0.01484
15	-2.31699	-1.39697	-0.14906	-2.30056	-1.39702	-0.14402
15	-2.20538	1.539385	0.058848	-2.1797	1.538142	0.091206
9	1.190958	-0.04224	-2.87676	1.198392	-0.04363	-2.88828
9	-1.17307	0.032393	-2.88256	-1.1819	0.03032	-2.89536
9	-1.37913	-0.8116	2.840372	-1.39502	-0.79502	2.85332
9	0.939357	-1.16664	3.040804	0.936687	-1.19039	3.057994
9	-2.794	2.197868	1.395422	-2.76907	2.189801	1.452863
9	-3.06822	2.441486	-0.94006	-3.04795	2.470517	-0.90049
9	-3.12906	-2.23657	0.939164	-3.11428	-2.26371	0.94659
9	-3.11181	-1.99335	-1.40321	-3.09387	-2.00344	-1.41468
6	-4.58226	0.138164	0.174818	-4.59343	0.166045	0.052502
1	-5.03491	-0.61257	-0.47875	-5.00181	0.25368	-0.9676
1	-4.85294	-0.06099	1.215694	-4.97951	-0.74472	0.536755
1	-4.95491	1.12121	-0.12281	-4.90371	1.034583	0.654993
6	0.242127	1.952363	3.090775	0.270966	1.978386	3.090903
1	-0.68422	2.536635	3.17265	-0.67696	2.542177	3.179081
1	0.371788	1.386295	4.021633	0.43289	1.419651	4.030946
1	1.087568	2.645523	3.002701	1.103065	2.696472	2.976861
6	0.04156	2.490826	-1.78575	0.015361	2.451185	-1.75802
6	0.12554	3.358782	0.412791	0.132363	3.32686	0.372189
6	-0.052	-2.69786	-1.62582	-0.04869	-2.67412	-1.5979
6	-0.13417	-3.16174	0.805024	-0.13948	-3.13536	0.789422
8	-0.1855	-4.18388	1.340124	-0.19549	-4.1809	1.311745
8	-0.05352	-3.45819	-2.5002	-0.04889	-3.44764	-2.4799
8	0.158544	4.467552	0.733176	0.170192	4.464291	0.648558
8	0.034954	3.134129	-2.75607	-0.00737	3.10197	-2.74217
7	3.103973	-0.10844	0.043541	3.105357	-0.10776	0.046246
15	2.33806	1.39858	-0.02628	2.317636	1.401014	-0.0272
15	2.208128	-1.54732	-0.06163	2.188591	-1.54755	-0.05283
9	3.022327	2.117317	1.229575	3.02215	2.145895	1.224803
9	3.242543	2.132464	-1.12213	3.208494	2.143007	-1.15144
9	2.913258	-2.37768	1.106992	2.897487	-2.39494	1.123257
9	2.998414	-2.27869	-1.24627	2.97657	-2.29307	-1.25209
6	4.584886	-0.18237	0.22584	4.596106	-0.18614	0.143452
1	4.83106	-0.31887	1.282755	4.878624	-0.79133	1.019976
1	4.979076	-1.01745	-0.35947	5.01054	-0.63055	-0.77636
1	5.040497	0.739493	-0.14383	5.002987	0.829256	0.266848

Table S97: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **S-34-1T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-3.11122	0.233518	-0.60813	3.11261	-0.24968	-0.58727
15	-2.13552	1.56029	-0.2656	2.08497	-1.56368	-0.23765
15	-2.33018	-1.27169	-0.75412	2.336098	1.258234	-0.7496
24	0.141957	1.306256	-0.57889	-0.13217	-1.2506	-0.56572
24	-0.12387	-1.45052	-0.25227	0.130058	1.422444	-0.24283
7	3.131129	-0.41748	-0.565	-3.11987	0.442116	-0.59721
15	2.086407	-1.56181	0.138204	-2.08119	1.557294	0.159749
15	2.359063	0.974536	-1.1011	-2.28279	-0.93195	-1.15475
9	-2.83443	2.674361	-1.1793	2.789599	-2.69954	-1.14983
9	-2.77315	2.090644	1.105472	2.719543	-2.09917	1.153016
9	-2.85051	-1.71717	-2.20128	2.8585	1.717301	-2.2076
9	-3.38158	-2.17195	0.052297	3.377175	2.188946	0.06642
9	2.777908	1.003919	-2.64436	-2.6482	-0.90169	-2.72848
9	3.414525	2.090051	-0.64891	-3.36878	-2.07265	-0.78188
9	2.841334	-2.89328	-0.34378	-2.80884	2.934482	-0.28377
9	2.673474	-1.60793	1.633858	-2.6711	1.574352	1.670742
6	4.608443	-0.57819	-0.62784	-4.59663	0.597928	-0.69505
1	5.083359	-0.12359	0.247255	-5.102	0.043302	0.113133
1	4.847598	-1.64358	-0.66858	-4.84662	1.668729	-0.6271
1	4.985177	-0.10382	-1.53885	-4.9364	0.222672	-1.67453
6	0.247168	3.0834	-1.29857	-0.27908	-2.99435	-1.25697
6	-0.25415	0.717722	-2.32253	0.332102	-0.7031	-2.29537
6	-0.35772	-3.21641	0.346306	0.385552	3.177822	0.373145
6	0.236214	-2.17197	-1.98201	-0.24699	2.114901	-1.96114
8	0.454349	-2.67658	-3.00071	-0.48221	2.615606	-2.99514
8	-0.50261	-4.32754	0.651	0.544133	4.295596	0.694349
8	-0.48486	0.472714	-3.43816	0.607844	-0.49075	-3.422
8	0.303845	4.146536	-1.74812	-0.36002	-4.07639	-1.70364
7	0.101241	0.540579	2.673803	-0.14827	-0.55996	2.680775
15	0.59431	1.756979	1.630644	-0.65651	-1.74877	1.588318
15	-0.50179	-0.86336	1.912105	0.504108	0.828393	1.915711
9	-0.04203	3.05198	2.324883	-0.05898	-3.08813	2.270498
9	2.083001	2.052078	2.148307	-2.17255	-2.02409	2.085949
9	-2.02395	-0.82051	2.43883	2.04012	0.753388	2.444235
9	-0.01007	-1.90948	3.027926	0.037525	1.903616	3.039632
6	0.137308	0.676422	4.153981	-0.20831	-0.70847	4.16044
1	0.972309	0.1044	4.568792	-1.03651	-0.11051	4.574552
1	0.248235	1.73255	4.414038	-0.35798	-1.77233	4.405733
1	-0.80505	0.314463	4.57588	0.747583	-0.38115	4.601896
6	-4.59387	0.344485	-0.69059	4.59529	-0.38305	-0.66047
1	-5.05292	0.058361	0.260427	5.056919	-0.13232	0.30887
1	-4.86513	1.373688	-0.939	4.848294	-1.41792	-0.94087
1	-4.95713	-0.30899	-1.4891	4.979866	0.290867	-1.4437

Table S98: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **S-34-2S** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	-2.04837	0.146013	-2.12539	-2.08187	0.118159	-2.10127
15	-1.75385	1.561576	-1.26838	-1.76766	1.535989	-1.23479
15	-0.93742	-1.10599	-1.7931	-0.89871	-1.08804	-1.78143
24	0.21569	1.443019	-0.17087	0.201264	1.396607	-0.18173
24	0.195944	-1.44437	0.168054	0.211558	-1.39071	0.183561
7	3.25538	-0.00953	-0.01436	3.282113	0.025475	-0.02407
15	2.293664	-1.24789	-0.65074	2.302822	-1.2354	-0.61397
15	2.316464	1.232081	0.643722	2.291706	1.24886	0.62215
9	-1.94706	2.669007	-2.40475	-1.97457	2.669128	-2.36635
9	-3.17263	1.841216	-0.57618	-3.18809	1.824052	-0.5118
9	-0.11353	-1.16859	-3.16397	-0.04072	-1.0777	-3.15142
9	-1.92085	-2.31817	-2.16603	-1.82606	-2.34868	-2.2073
9	3.292458	2.471496	0.36155	3.244631	2.525171	0.330709
9	2.663102	1.14499	2.202791	2.630918	1.189498	2.200252
9	2.634885	-1.17244	-2.21158	2.645844	-1.22564	-2.19205
9	3.268179	-2.48692	-0.36098	3.276441	-2.48483	-0.27597
6	4.739742	-0.05283	-0.00707	4.768151	0.010129	-0.02129
1	5.100898	-0.76082	0.745328	5.153195	-0.5459	0.850267
1	5.100742	-0.35212	-0.99606	5.126443	-0.46585	-0.9489
1	5.123961	0.945738	0.214163	5.136972	1.047837	0.004628
6	0.20336	3.229802	0.354262	0.186113	3.171385	0.336392
6	1.067248	2.065471	-1.75041	1.036311	2.022885	-1.74911
6	1.049681	-2.06402	1.746894	1.045049	-1.99432	1.760529
6	0.173242	-3.232	-0.35378	0.214793	-3.16856	-0.3247
8	0.180185	-4.36762	-0.60527	0.239487	-4.31973	-0.57421
8	1.569729	-2.49447	2.688603	1.56382	-2.42519	2.720499
8	1.586044	2.496241	-2.69246	1.557014	2.466479	-2.70216
8	0.218761	4.364969	0.607364	0.201506	4.321286	0.592343
7	-2.043	-0.12577	2.129279	-2.09296	-0.13478	2.090354
15	-0.91267	1.109066	1.794226	-0.91752	1.080619	1.776215
15	-1.77156	-1.5465	1.274003	-1.76188	-1.55015	1.226531
9	-1.87631	2.334308	2.176649	-1.85801	2.333113	2.197497
9	-0.08087	1.154304	3.161059	-0.06567	1.078896	3.150039
9	-3.19723	-1.80999	0.590283	-3.17589	-1.85182	0.496977
9	-1.97083	-2.65055	2.412362	-1.96296	-2.6851	2.357053
6	-3.12406	0.034682	3.137925	-3.2046	0.027214	3.06672
1	-2.70479	0.416377	4.073908	-2.8077	0.372025	4.036073
1	-3.88832	0.723176	2.766558	-3.9431	0.750916	2.685446
1	-3.57515	-0.94193	3.33247	-3.69014	-0.95094	3.21442
6	-3.13462	0.001774	-3.13086	-3.1852	-0.05154	-3.08572
1	-3.9093	-0.67328	-2.75637	-3.9212	-0.78077	-2.71017
1	-3.56979	0.985376	-3.32627	-3.67678	0.92311	-3.23653
1	-2.72403	-0.38864	-4.06711	-2.77877	-0.39294	-4.05234

Table S99: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ structure **S-34-2T** at B3LYP/DZP and BP86/DZP levels.

Atomic Number	B3LYP			BP86		
	X	Y	Z	X	Y	Z
7	0.000003	1.038551	1.784044	-3.1E-05	1.035912	1.791615
15	-1E-06	0.004878	-1.592	0.000005	0.012941	-1.59025
15	-1E-06	-0.58601	1.853901	0.000005	-0.61871	1.855912
24	0.000005	1.809507	-0.111	-1.8E-05	1.772963	-0.09612
24	-8E-06	-1.71985	-0.16007	0.000016	-1.70624	-0.15032
7	-3.05052	-0.03365	0.02084	-3.03819	-0.02132	0.02151
15	-2.24128	-1.55562	-0.14286	-2.22808	-1.54885	-0.14065
15	-2.33769	1.492069	-0.02515	-2.29067	1.506641	-0.0206
9	1.192681	0.09672	-2.68825	1.197564	0.087661	-2.6999
9	-1.19267	0.096722	-2.68826	-1.19756	0.087632	-2.6999
9	-1.17763	-0.97052	2.892641	-1.18899	-0.98671	2.908335
9	1.177636	-0.97052	2.892629	1.189025	-0.98666	2.908323
9	-3.03834	2.170881	1.240976	-3.01119	2.193921	1.254518
9	-3.22804	2.227461	-1.12808	-3.17652	2.258348	-1.13836
9	-3.07593	-2.34608	0.96991	-3.0695	-2.35274	0.980786
9	-3.07428	-2.12957	-1.38292	-3.06096	-2.13827	-1.39393
6	-4.53885	-0.08432	0.207432	-4.52977	-0.05864	0.196642
1	-4.95805	-0.84467	-0.4562	-4.95278	-0.82483	-0.47234
1	-4.77901	-0.32068	1.247388	-4.78422	-0.28793	1.243699
1	-4.97643	0.879833	-0.06084	-4.95783	0.916	-0.08448
6	-4E-06	1.836066	3.029266	-4.5E-05	1.831851	3.038122
6	-0.89217	2.472267	3.074455	-0.8979	2.475148	3.073103
6	-2.6E-05	1.194441	3.917713	-8.3E-05	1.184832	3.932933
6	0.892181	2.472244	3.074482	0.897827	2.475116	3.073149
8	0.000008	2.853648	-1.77647	-0.00001	2.798508	-1.70462
8	0.000015	3.587573	0.643819	-0.00004	3.536285	0.601202
8	-7E-06	-2.84797	-1.67844	0.000018	-2.81213	-1.66879
8	-1.5E-05	-3.35123	0.826484	0.000039	-3.34738	0.783213
7	-1.7E-05	-4.38157	1.354332	0.000059	-4.4114	1.276519
15	-7E-06	-3.56948	-2.58508	0.000018	-3.53893	-2.58858
15	0.000026	4.686682	1.003115	-5.3E-05	4.6729	0.895664
9	0.000009	3.485598	-2.73785	-7E-06	3.476593	-2.65722
9	3.050514	-0.03367	0.020862	3.038187	-0.02126	0.021553
9	2.337702	1.492053	-0.02516	2.290642	1.506681	-0.02061
9	2.24127	-1.55563	-0.14286	2.22811	-1.54881	-0.14064
6	3.038366	2.170879	1.240958	3.011167	2.194019	1.254473
1	3.228054	2.227417	-1.1281	3.176451	2.258367	-1.13841
1	3.07592	-2.34612	0.969886	3.069544	-2.35269	0.98079
1	3.07425	-2.12957	-1.38294	3.061008	-2.13819	-1.39392
6	4.538842	-0.08435	0.207473	4.529767	-0.05856	0.196695
1	4.778987	-0.32069	1.247436	4.784203	-0.28793	1.243738
1	4.958047	-0.84472	-0.45614	4.952798	-0.82469	-0.47234
1	4.976434	0.879789	-0.06081	4.957809	0.91611	-0.08434

Table S100: Atomic coordinates for the $[MeN(PF_2)_2]Cr_2(CO)_{10}$ open-shell singlet structure **110-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	-0.045113	-1.010256	0.707261
15	-1.665766	-1.289233	0.225548
15	1.224759	-0.823122	-0.387907
24	3.180544	0.274904	0.040559
24	-3.087798	0.437599	-0.065131
9	0.390675	-0.319755	-1.650456
9	1.394997	-2.307395	-0.911044
9	-1.405598	-2.287458	-0.96291
9	-2.060148	-2.359807	1.323915
6	3.580198	-0.956844	1.440614
6	2.407483	1.504112	1.280081
6	4.854558	1.125361	0.287519
6	2.748614	1.500029	-1.367378
6	4.005098	-0.892752	-1.229884
6	-1.576424	1.587331	-0.025574
6	-3.262124	0.574118	1.827993
6	-4.538263	-0.812205	-0.108475
6	-2.883069	0.269818	-1.964516
6	-4.275681	1.906843	-0.298601
8	3.821154	-1.695059	2.283719
8	2.480566	2.231183	-2.203677
8	5.868693	1.63459	0.435848
8	4.511655	-1.580249	-1.990163
8	1.976453	2.264929	2.020052
8	-4.987539	2.791153	-0.435601
8	-5.396001	-1.568283	-0.129469
8	-2.743305	0.161866	-3.093197
8	-3.351758	0.646765	2.967996
8	-0.617898	2.217135	0.007389
6	0.092753	-0.541421	2.092989
1	-0.427192	-1.222777	2.764895
1	1.142475	-0.537126	2.374411
1	-0.304664	0.468091	2.227659

Table S101: Atomic coordinates for the $[MeN(PF_2)_2]Cr_2(CO)_9$ open-shell singlet structure **19-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	-0.091653	2.165809	0.017116
15	-1.596558	1.448992	0.065628
15	1.44368	1.395912	-0.029052
24	-2.214565	-0.759097	0.038278
24	2.252895	-0.705221	0.066564
6	-0.091512	3.641862	-0.140316
1	0.811749	4.049626	0.304275
1	-0.132583	3.914367	-1.193458
1	-0.948769	4.066362	0.376856
9	-2.308273	2.27808	-1.090953
9	-2.260314	2.272952	1.252282
9	2.147595	2.34766	1.03518
9	1.974983	2.183644	-1.3066
6	3.825773	0.1799	-0.257499
6	1.953917	-0.876608	-1.813335
6	2.516193	-0.49587	1.952634
6	3.304074	-2.288621	0.074632
6	-1.886466	-0.785946	-1.849751
6	-3.995902	-0.085214	-0.271526
6	-2.511904	-0.674819	1.927728
6	-2.928595	-2.512869	-0.031018
8	4.824645	0.721014	-0.458061
8	2.714313	-0.339945	3.069628
8	1.819087	-0.939638	-2.949974
8	4.003013	-3.195204	0.062553
8	-2.67856	-0.623498	3.05689
8	-5.056483	0.295404	-0.452316
8	-1.685553	-0.806232	-2.974637
8	-3.357248	-3.572413	-0.072073
6	-0.537146	-1.500327	0.350417
8	0.467775	-2.048355	0.551325

Table S102: Atomic coordinates for the $[MeN(PF_2)_2]Cr_2(CO)_8$ open-shell singlet structure **18-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	0.006292	2.432739	0.028583
15	1.433927	1.548	0.042322
15	-1.425078	1.555671	-0.01614
6	0.011192	3.901492	-0.027109
1	-0.893497	4.286413	0.439436
1	0.870532	4.283912	0.520369
1	0.058774	4.248067	-1.05915
9	-2.172564	2.316917	-1.192306
9	-2.226264	2.281049	1.144466
9	2.218769	2.287867	-1.120827
9	2.204915	2.287185	1.216973
24	1.390847	-0.725491	-0.019532
24	-1.394752	-0.719857	0.016448
6	-0.422605	-0.64831	1.665915
6	-2.835799	-0.702729	1.176016
6	1.451497	-2.623381	-0.063165
6	-1.464682	-2.617325	0.025702
6	-2.708667	-0.710266	-1.384688
6	0.418978	-0.612135	-1.666465
6	2.833204	-0.698429	-1.177429
6	2.702393	-0.742488	1.384191
8	3.715413	-0.686864	-1.914187
8	3.522137	-0.744868	2.179421
8	0.104447	-0.516559	-2.774808
8	1.574074	-3.760037	-0.121552
8	-1.592183	-3.754435	0.062571
8	-3.530261	-0.699829	-2.178051
8	-3.717301	-0.697361	1.913662
8	-0.108282	-0.583799	2.776442

Table S103: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_8$ open-shell singlet structure **28-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
15	-0.00199	-1.887012	2.200432
15	-0.002413	1.173913	2.093687
24	-0.018761	-2.14246	0
24	-0.004045	2.314686	0
15	-0.002413	1.173913	-2.093687
15	-0.00199	-1.887012	-2.200432
6	1.243833	-3.57098	0
6	-1.298394	-3.556892	0
6	1.503187	-1.020228	0
6	1.908723	2.363388	0
6	-1.536707	-1.010963	0
6	-0.010655	3.732249	-1.212716
6	-1.917915	2.358719	0
8	-0.016885	4.657793	-1.893144
8	-3.054979	2.480166	0
8	-2.551765	-0.470931	0
8	3.046317	2.483637	0
8	2.518105	-0.479429	0
8	1.976217	-4.449491	0
8	-2.040106	-4.427479	0
6	-0.010655	3.732249	1.212716
8	-0.016885	4.657793	1.893144
9	1.160814	-2.559479	3.048094
9	-1.184536	-2.514368	3.055937
9	1.150099	1.83383	2.971864
9	-1.215508	1.771994	2.934896
9	1.160814	-2.559479	-3.048094
9	-1.184536	-2.514368	-3.055937
9	1.150099	1.83383	-2.971864
9	-1.215508	1.771994	-2.934896
7	0.050637	-0.346957	2.874537
7	0.050637	-0.346957	-2.874537
6	0.181276	-0.294976	-4.351713
1	1.230255	-0.287874	-4.642481
1	-0.309524	-1.161116	-4.789413
1	-0.305281	0.598686	-4.733256
6	0.181276	-0.294976	4.351713
1	-0.309524	-1.161116	4.789413
1	1.230255	-0.287874	4.642481
1	-0.305281	0.598686	4.733256

Table S104: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_7$ open-shell singlet structure **27-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	3.020293	0.398667	0.067227
15	2.421334	-1.137387	0.417559
15	1.948626	1.608376	-0.416423
24	0.253563	-1.476669	0.011126
24	-0.267603	1.492889	0.000127
7	-3.035845	-0.411581	0.054369
15	-2.432955	1.110871	0.418922
15	-1.950898	-1.622389	-0.419054
9	3.468128	-2.020307	-0.383295
9	3.086973	-1.382319	1.835049
9	2.43358	1.861843	-1.906426
9	2.725466	2.849556	0.198117
9	-2.460508	-1.898214	-1.897033
9	-2.714928	-2.857951	0.222918
9	-3.500309	2.010832	-0.334863
9	-3.050433	1.338202	1.862046
6	-4.476721	-0.697717	0.138478
1	-4.713512	-1.225345	1.061861
1	-5.033934	0.235804	0.106401
1	-4.782689	-1.30652	-0.710861
6	4.463505	0.680033	0.136313
1	4.769331	1.274393	-0.723373
1	4.709346	1.218323	1.051
1	5.014669	-0.257264	0.113988
6	-0.093406	-2.3259	1.669709
6	0.146852	0.173054	1.544189
6	0.519965	-3.246027	-0.476397
6	0.787151	-1.203044	-1.803063
6	-0.732573	0.97418	-1.786783
6	-0.546363	3.185197	-0.746713
6	-0.085482	2.591867	1.526808
8	-0.721097	4.229797	-1.187484
8	0.005614	3.295431	2.424516
8	-1.093543	0.83915	-2.867635
8	0.692047	-4.344028	-0.770791
8	-0.273331	-2.916773	2.634385
8	0.322998	0.146759	2.696346
8	1.18003	-1.192206	-2.881734

Table S105: Atomic coordinates for the $[MeN(PF_2)_2]_2Cr_2(CO)_6$ open-shell singlet structure **26-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	-3.13778	-0.001186	0.011579
15	-2.247433	-1.425093	-0.00739
15	-2.248237	1.423579	0.010919
24	0	-1.377727	0.014808
24	0	1.37847	0.003898
7	3.137779	-0.001185	0.011579
15	2.248235	1.423579	0.010916
15	2.247433	-1.425092	-0.007387
9	-3.029036	-2.248028	1.104315
9	-2.945705	-2.161959	-1.228443
9	-2.954154	2.185423	1.211492
9	-3.026326	2.219975	-1.123205
9	3.029035	-2.248024	1.104322
9	2.945707	-2.161962	-1.228437
9	2.954154	2.185427	1.211487
9	3.026323	2.219973	-1.123211
6	4.604061	0.001773	-0.062292
1	4.93896	0.041665	-1.09869
1	4.99512	0.864266	0.474342
1	4.994011	-0.900369	0.405175
6	-4.604061	0.001772	-0.062291
1	-4.99512	0.864263	0.474345
1	-4.938961	0.041666	-1.098689
1	-4.994011	-0.900371	0.405173
6	0.000001	-2.848259	-1.103111
6	0.000001	-0.449842	-1.649463
6	-0.000001	-2.656052	1.444612
6	-0.000001	2.665867	-1.416205
6	0.000001	0.448073	1.668268
6	0	2.843083	1.129004
8	0	0.154392	2.788725
8	0	3.740495	1.849345
8	-0.000003	3.474518	-2.223928
8	0	-3.458606	2.25814
8	0.000002	-3.749381	-1.818904
8	0.000004	-0.151774	-2.768954

Table S106: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_6$ open-shell singlet structure **36-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
24	2.276287	0.058011	-0.456606
24	-2.299866	0.312926	0.342112
7	0.032897	2.79014	-0.527679
15	-1.212579	1.751849	-1.029347
15	1.391175	2.065026	0.131207
9	1.22223	2.408657	1.680657
9	2.413531	3.247413	-0.15546
9	-2.165906	2.895706	-1.574515
9	-0.693412	1.284091	-2.461561
7	0.592712	-0.923805	2.502645
15	-0.994952	-0.818779	1.89925
15	2.024602	-0.715832	1.644786
9	2.709415	-2.121454	1.93701
9	2.840388	0.065166	2.76318
9	-1.313904	-2.383348	1.843715
9	-1.664403	-0.569759	3.321973
6	0.730596	-1.466048	3.877947
1	0.519072	-0.691328	4.611958
1	0.046641	-2.30007	4.022674
1	1.744817	-1.826884	4.022683
7	-0.691164	-1.950851	-1.839853
15	0.904582	-1.601888	-1.357719
15	-2.110269	-1.328427	-1.192452
9	-2.860283	-2.686728	-0.847986
9	-2.892107	-1.081376	-2.554806
9	1.204117	-2.987896	-0.619166
9	1.560631	-2.015462	-2.747049
6	-0.849796	-3.04037	-2.834472
1	-0.635426	-2.672728	-3.835966
1	-0.178519	-3.863698	-2.598424
1	-1.869793	-3.412724	-2.801368
6	-0.176196	4.2479	-0.450835
1	-1.129233	4.478214	0.022377
1	0.618652	4.689124	0.144155
1	-0.156215	4.690035	-1.446065
6	-3.595003	-0.665067	1.289693
6	3.499406	-1.3126	-0.839841
8	-4.445826	-1.228149	1.814253
8	4.316677	-2.091778	-1.043514
6	-3.82606	0.917613	-0.557139
8	-4.798883	1.249696	-1.066655
6	2.439185	0.780942	-2.191367
8	2.54277	1.235682	-3.239255
6	3.854273	0.894627	0.092698
8	4.86011	1.346337	0.411873
6	-2.373764	1.747735	1.557635
8	-2.403861	2.637771	2.28384

Table S107: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_5$ open-shell singlet structure **35-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	-2.824176	1.211057	-0.447939
15	-1.46817	2.086693	0.047019
15	-2.629824	-0.412881	-0.848312
24	0.607707	1.384916	-0.41806
24	-0.636753	-1.35934	-0.468034
7	2.790074	-1.183764	-0.609963
15	1.453132	-2.069234	-0.086836
15	2.573157	0.455443	-0.936828
9	-1.88156	3.506519	-0.534233
9	-1.89329	2.441215	1.543577
9	-3.259637	-0.430938	-2.303372
9	-3.915204	-1.009679	-0.137726
9	3.127434	0.530078	-2.421217
9	3.894346	1.025842	-0.270958
9	1.851318	-3.479225	-0.699959
9	1.92187	-2.444508	1.39497
6	4.143694	-1.755928	-0.586255
1	4.638621	-1.538571	0.361252
1	4.086338	-2.832711	-0.724877
1	4.73153	-1.33463	-1.400157
6	-0.074264	0.056129	-1.973487
6	1.406386	2.980634	0.099698
6	0.528433	2.40217	-1.987586
6	-1.436581	-2.973143	-0.008253
6	-0.574188	-2.306799	-2.081506
8	-0.558468	-2.940655	-3.036557
8	-1.94416	-3.978705	0.223121
8	0.507664	3.077243	-2.913593
8	-0.119825	0.098203	-3.140105
8	1.908684	3.980701	0.364912
7	0.09633	-0.098214	2.694056
15	1.02703	0.936049	1.770067
15	-0.938491	-1.021333	1.756715
9	1.009703	2.202367	2.729135
9	2.495336	0.486392	2.204439
9	-2.361203	-0.537109	2.291787
9	-0.921384	-2.338208	2.645175
6	0.235945	-0.257878	4.142998
1	0.854091	-1.126082	4.373257
1	0.696645	0.634443	4.561365
1	-0.74545	-0.385506	4.597213
6	-4.174098	1.784863	-0.347326
1	-4.625422	1.544074	0.616004
1	-4.119679	2.864754	-0.460674
1	-4.800365	1.386503	-1.144045

Table S108: Atomic coordinates for the $[MeN(PF_2)_2]_3Cr_2(CO)_4$ open-shell singlet structure **34-1S** at M06-L/TZP level.

Atomic Number	uM06-L		
	X	Y	Z
7	0.403118	1.037833	1.978167
15	0.029612	-0.003642	-1.773897
15	-0.106418	-0.458458	1.952011
24	0.089632	1.482829	-0.133945
24	-0.060683	-1.479567	-0.128555
7	-3.075952	0.126604	-0.054652
15	-2.291345	-1.352353	-0.200522
15	-2.148413	1.515647	0.10808
9	1.214263	-0.037627	-2.830433
9	-1.118371	0.042936	-2.86798
9	-1.54953	-0.538041	2.669071
9	0.628472	-1.24982	3.129396
9	-2.760439	2.118773	1.446209
9	-2.964017	2.472673	-0.860037
9	-3.131256	-2.208546	0.836587
9	-3.041444	-1.924785	-1.477822
6	-4.543637	0.208544	-0.087674
1	-4.895619	0.409101	-1.099376
1	-4.968772	-0.729672	0.261904
1	-4.880434	1.004204	0.574668
6	0.365933	1.934609	3.114009
1	-0.602779	2.435371	3.216003
1	0.562688	1.398375	4.045484
1	1.132632	2.70485	3.011367
6	-0.018821	2.358759	-1.745386
6	0.192762	3.289662	0.42253
6	-0.002881	-2.633557	-1.602042
6	-0.205406	-3.081762	0.869856
8	-0.297976	-4.063643	1.44862
8	0.037953	-3.348084	-2.499397
8	0.253112	4.392749	0.720233
8	-0.083504	2.952701	-2.73533
7	3.097947	-0.142413	0.062464
15	2.345121	1.346901	-0.08531
15	2.157543	-1.53897	0.024256
9	3.093256	2.146867	1.062526
9	3.190488	1.974963	-1.270898
9	2.812695	-2.323011	1.238131
9	2.957312	-2.341232	-1.092701
6	4.565695	-0.238854	0.092444
1	4.864255	-1.079835	0.715013
1	4.964311	-0.374547	-0.912731
1	4.980239	0.670289	0.522674

Table S109: The energies (E, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the lowest-energy open-shell singlet structures of $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=1, n=10, 9, 8) using M06-L /TZP method.

Singlet		**110-1S(C_1)**	**19-1S(C_1)**	**18-1S(C_1)**
uM06-L	E	-4399.819755	-4286.423658	-4173.044978
	Nimg	0	0	0

Table S110: The energies (E, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the lowest-energy open-shell singlet structures of $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=2, n=8, 7, 6) using M06-L /TZP method.

Singlet		**28-1S(C_S)**	**27-1S(C_1)**	**26-1S(C_S)**
uM06-L	E	-5350.126305	-5236.756710	-5123.382333
	Nimg	0	0	0

Table S111: The energies (E, in kcal mol^{-1}), numbers of imaginary vibrational frequencies (Nimg) for the lowest-energy open-shell singlet structures of $[MeN(PF_2)_2]_mCr_2(CO)_n$ (m=3, n=6, 5, 4) using M06-L /TZP method.

Singlet		**36-1S(C_1)**	**35-1S(C_1)**	**34-1S(C_1)**
uM06-L	E	-6300.457948	-6187.096022	-6073.729736
	Nimg	0	0	0

Figure S10: The frontier molecular orbital graphs of the two unpaired electrons in the open-shell triplet structure **18-1T.**

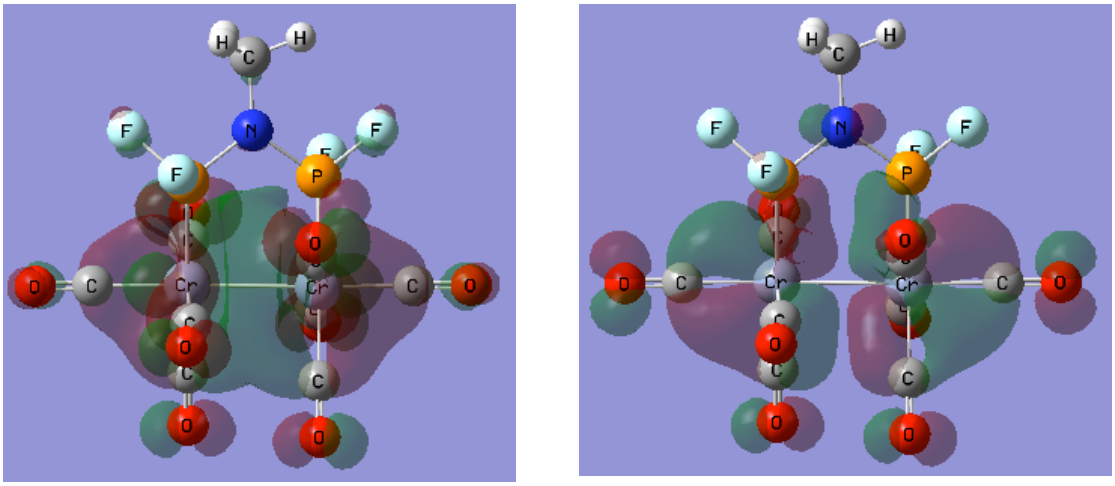


Figure S11: The frontier molecular orbital graphs of the two unpaired electrons in the open-shell triplet structure **18-2T.**

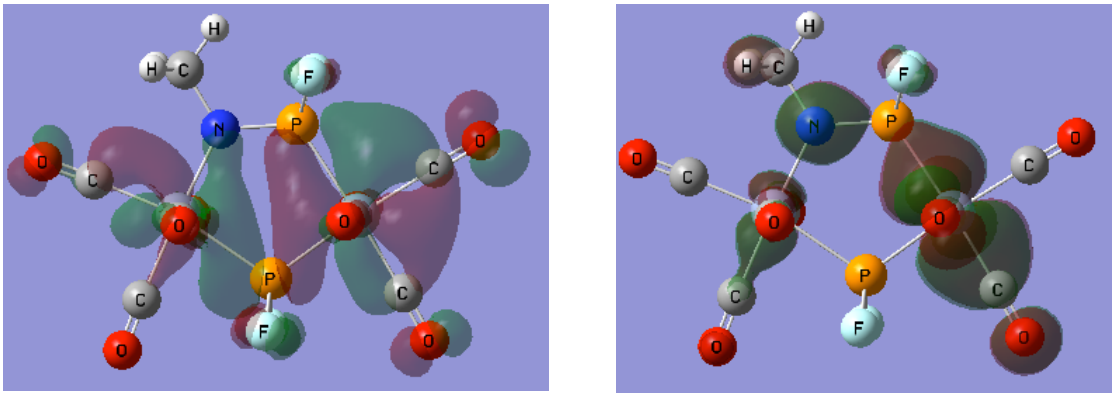


Figure S12: The frontier molecular orbital graphs of the two unpaired electrons in the open-shell triplet structure **34-1T.**

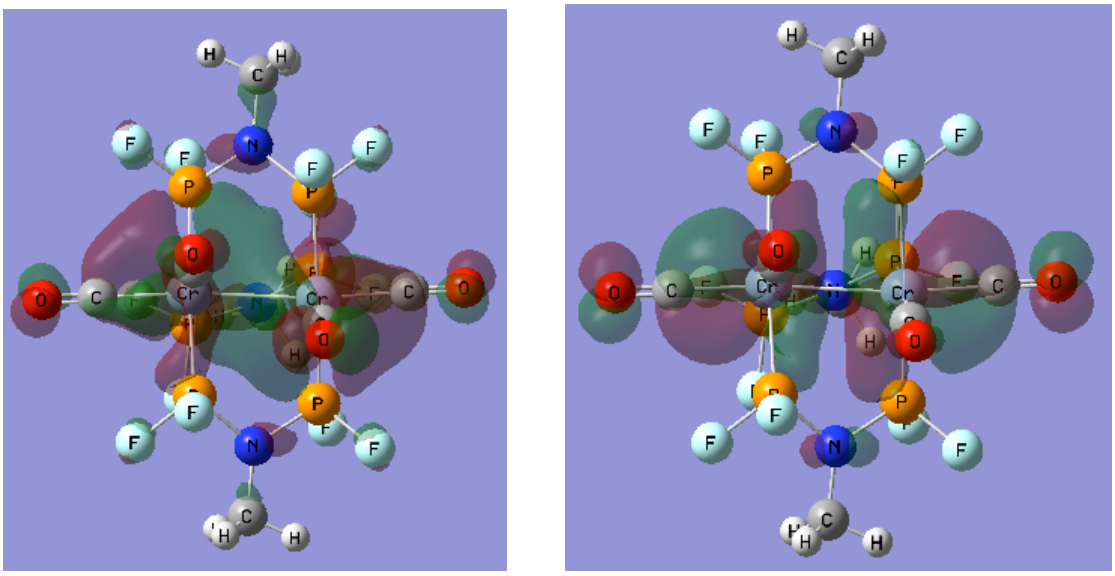


Figure S13: The frontier molecular orbital graphs of the two unpaired electrons in the open-shell triplet structure **34-2T.**