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I in the closed-shell singlet state SCF = -4240.81103875

Mo	2.038552	2.015563	0.141606
Mo	0.534244	-2.675979	-0.258604
I	4.609013	1.965057	1.429941
I	2.343289	-4.199756	-1.843062
P	2.745885	2.107028	-2.155836
P	1.061188	3.462922	2.019527
P	1.493879	-3.387955	1.868884
P	-1.362429	-2.525273	-1.943544
N	1.373092	0.250655	0.075140
N	0.982790	-0.890715	-0.004117
N	0.229663	2.845612	-0.775463
N	-1.179871	-2.817886	1.026130
C	1.250391	2.844825	-3.026230
C	0.031373	2.923941	-2.139981
C	-1.220919	3.128035	-2.704146
C	-2.361281	3.348301	-1.904554
C	-2.091602	3.499635	-0.535896
C	-0.849701	3.216721	-0.003392
C	-0.707562	3.240456	1.495998
C	4.125215	3.366683	-2.640162
C	4.094339	3.830342	-4.112547
C	3.917985	4.609121	-1.748272
C	5.512331	2.771132	-2.330075
C	3.067866	0.438586	-3.050652
C	1.700682	-0.252236	-3.221486
C	3.701859	0.533136	-4.450327
C	3.962464	-0.423277	-2.133653
C	1.358151	5.348429	1.989375
C	0.908415	5.856744	0.601360
C	0.581786	6.123962	3.067203
C	2.870375	5.611949	2.139925
C	1.023442	2.785427	3.804991
C	-0.227498	3.191941	4.610638
C	2.294675	3.203329	4.569035

C	1.029716	1.251730	3.647393
C	0.301048	-2.373825	2.932174
C	-1.085871	-2.440540	2.344704
C	-2.225583	-2.089027	3.067615
C	-3.500763	-2.205222	2.485811
C	-3.567151	-2.867058	1.248124
C	-2.416938	-3.140142	0.532794
C	-2.437089	-3.665010	-0.860570
C	1.110243	-5.233272	2.301801
C	2.319716	-6.121123	1.942406
C	0.710621	-5.432214	3.776284
C	-0.066090	-5.724214	1.425039
C	3.221986	-2.934585	2.560722
C	3.302116	-1.399547	2.633703
C	4.287049	-3.396571	1.542496
C	3.531729	-3.485262	3.964813
C	-1.475963	-3.468860	-3.625719
C	-0.385129	-2.898200	-4.555466
C	-1.163585	-4.961902	-3.373694
C	-2.848376	-3.411329	-4.322960
C	-2.457898	-0.927750	-2.044910
C	-2.089786	-0.117636	-3.303310
C	-3.978363	-1.190744	-2.042310
C	-2.133893	-0.052789	-0.813523
H	1.505881	3.877663	-3.290549
H	1.023016	2.339470	-3.969265
H	-1.312057	3.058311	-3.783578
H	-2.881577	3.778170	0.152307
H	-1.399740	3.969246	1.933238
H	-0.990178	2.255985	1.890659
H	3.151228	4.314621	-4.387220
H	4.277395	3.019964	-4.818321
H	4.887853	4.575282	-4.259414
H	5.770943	1.955580	-3.010089
H	5.577309	2.400983	-1.304592
H	6.274089	3.552899	-2.453120

H	2.936106	5.072609	-1.901666
H	4.678572	5.363343	-1.992307
H	4.025489	4.362837	-0.688295
H	1.075380	-0.181796	-2.332624
H	1.145014	0.159828	-4.071458
H	1.861933	-1.315898	-3.416169
H	3.114340	1.164753	-5.127037
H	3.729728	-0.473716	-4.887832
H	4.728719	0.905763	-4.429054
H	4.124229	-1.401545	-2.602477
H	4.936873	0.039325	-1.952600
H	3.493373	-0.597759	-1.163496
H	1.383283	5.298307	-0.210232
H	-0.175944	5.791228	0.466359
H	1.194545	6.911520	0.500264
H	-0.495501	5.927689	3.024471
H	0.724734	7.200778	2.906121
H	0.936052	5.896780	4.076131
H	3.058911	6.688391	2.033186
H	3.256141	5.300270	3.112929
H	3.451594	5.084531	1.379343
H	-1.155688	2.854528	4.137848
H	-0.299003	4.269161	4.772768
H	-0.177012	2.715073	5.598609
H	2.300785	4.272690	4.800912
H	2.327334	2.663640	5.524784
H	3.204587	2.957203	4.012899
H	1.039432	0.781971	4.640344
H	1.914356	0.919398	3.101408
H	0.143201	0.884399	3.117271
H	0.689161	-1.355600	2.836995
H	0.280474	-2.618035	4.000673
H	-2.110123	-1.656271	4.057069
H	-4.528834	-3.091604	0.800512
H	-3.455967	-3.787275	-1.236892
H	-1.951345	-4.645902	-0.896056

H	2.617409	-5.982466	0.897480
H	2.038249	-7.174443	2.073693
H	3.186996	-5.937338	2.579136
H	1.476614	-5.092998	4.476171
H	0.541193	-6.501022	3.964854
H	-0.223623	-4.909872	4.011861
H	-1.005049	-5.217989	1.658427
H	-0.217160	-6.797058	1.605582
H	0.149333	-5.604306	0.356058
H	2.973728	-0.913402	1.713875
H	4.343464	-1.098430	2.792205
H	2.724102	-1.001635	3.472049
H	4.311739	-4.477670	1.397195
H	5.275698	-3.084235	1.903665
H	4.121785	-2.935040	0.565301
H	2.781009	-3.170083	4.699234
H	4.498640	-3.083535	4.296054
H	3.606681	-4.574723	3.994631
H	-0.514149	-1.830020	-4.749004
H	-0.424429	-3.418759	-5.522094
H	0.609485	-3.054141	-4.130310
H	-0.264854	-5.110090	-2.771573
H	-0.987381	-5.449979	-4.340993
H	-2.004056	-5.482226	-2.900897
H	-3.649817	-3.795275	-3.682231
H	-2.815729	-4.048531	-5.217085
H	-3.123077	-2.407495	-4.653167
H	-1.028981	0.141584	-3.318699
H	-2.658312	0.818351	-3.299428
H	-2.332586	-0.640508	-4.230456
H	-4.313740	-1.816219	-2.870688
H	-4.500067	-0.227796	-2.124870
H	-4.308296	-1.653890	-1.108339
H	-2.319096	-0.569593	0.131048
H	-2.778564	0.831935	-0.840614
H	-1.099011	0.289463	-0.811663

C	-6.578311	-0.039528	2.377499
C	-6.934144	0.037930	3.734373
C	-6.186398	-0.644074	4.699065
C	-5.066167	-1.399956	4.344888
C	-4.705574	-1.513537	2.993754
C	-5.485835	-0.844916	2.037723
H	-7.766661	0.665145	4.040755
H	-6.469800	-0.566998	5.745351
H	-4.485850	-1.910684	5.108675
H	-5.199376	-0.919798	0.995571
C	-8.358847	2.316924	-0.757099
C	-9.158679	1.827073	0.278312
C	-8.613362	1.060524	1.310867
C	-7.242429	0.759524	1.312124
C	-6.460526	1.251816	0.258284
C	-6.982851	2.039061	-0.777726
H	-8.798006	2.940046	-1.531132
H	-10.221934	2.051836	0.283815
H	-9.254427	0.678207	2.100428
H	-5.402248	1.021980	0.250528
C	-5.479473	3.201643	-4.087994
C	-6.430608	2.765748	-3.160085
C	-6.058702	2.565162	-1.819699
C	-4.732876	2.831353	-1.464478
C	-3.750835	3.246976	-2.381505
C	-4.153305	3.432107	-3.718097
H	-5.775611	3.349253	-5.123285
H	-7.443842	2.547161	-3.484820
H	-4.443520	2.675039	-0.434523
H	-3.436605	3.765928	-4.463144

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I in the triplet state SCF = -4240.81945180

Mo	1.973449	2.178277	0.183224
Mo	0.642198	-2.570010	-0.276262
I	4.576559	2.081657	1.410534

I	2.480298	-4.068828	-1.903401
P	2.706897	2.229042	-2.169024
P	0.894588	3.256369	2.132501
P	1.614634	-3.364304	1.833021
P	-1.286302	-2.505356	-1.987947
N	1.282852	0.411038	0.213710
N	0.955486	-0.740511	0.104284
N	0.140331	2.944283	-0.749161
N	-1.058605	-2.787084	0.983526
C	1.191712	3.007925	-2.990303
C	-0.036875	3.027637	-2.111619
C	-1.297728	3.169477	-2.686379
C	-2.447173	3.334140	-1.892385
C	-2.205906	3.465364	-0.517383
C	-0.961591	3.212415	0.026458
C	-0.860861	3.139661	1.528216
C	4.064665	3.502625	-2.649037
C	4.017484	3.991604	-4.111859
C	3.850705	4.721027	-1.722587
C	5.457739	2.910024	-2.359492
C	2.997558	0.572447	-3.067695
C	1.623249	-0.105384	-3.204558
C	3.613883	0.663924	-4.474377
C	3.896799	-0.285702	-2.151244
C	1.205784	5.152418	2.246348
C	0.811340	5.777462	0.888347
C	0.388335	5.849977	3.347250
C	2.707184	5.421364	2.474224
C	0.741706	2.500136	3.883810
C	-0.513741	2.904672	4.682074
C	2.014698	2.814846	4.691594
C	0.689484	0.980388	3.642032
C	0.396326	-2.431248	2.930479
C	-0.985785	-2.486211	2.328891
C	-2.134937	-2.194313	3.061608
C	-3.407704	-2.305047	2.470851

C	-3.446886	-2.935164	1.212916
C	-2.290441	-3.153920	0.494801
C	-2.298018	-3.673732	-0.901676
C	1.288469	-5.234516	2.185575
C	2.520847	-6.073937	1.791070
C	0.903797	-5.499788	3.654260
C	0.118344	-5.720689	1.298591
C	3.332990	-2.875824	2.524438
C	3.368398	-1.340748	2.648485
C	4.403785	-3.272223	1.485057
C	3.667049	-3.465699	3.906773
C	-1.368941	-3.447631	-3.670979
C	-0.300683	-2.839981	-4.602405
C	-1.007044	-4.929673	-3.420888
C	-2.744697	-3.433827	-4.363554
C	-2.433431	-0.945241	-2.082722
C	-2.109601	-0.115688	-3.340039
C	-3.943014	-1.268013	-2.071067
C	-2.136561	-0.066363	-0.848183
H	1.449185	4.054899	-3.187497
H	0.966783	2.565136	-3.965511
H	-1.381387	3.093847	-3.765779
H	-3.017162	3.685861	0.165874
H	-1.550574	3.857461	1.987698
H	-1.192700	2.140405	1.836633
H	3.068727	4.473736	-4.370573
H	4.196853	3.190139	-4.829605
H	4.805814	4.742296	-4.256847
H	5.714909	2.108645	-3.057171
H	5.532075	2.521784	-1.341096
H	6.213797	3.698460	-2.474162
H	2.859311	5.174984	-1.847143
H	4.592931	5.495254	-1.958824
H	3.985258	4.452559	-0.669562
H	1.033561	-0.046509	-2.289375
H	1.040809	0.328159	-4.025277

H	1.772336	-1.165586	-3.425142
H	3.017897	1.293850	-5.145394
H	3.639745	-0.343944	-4.909290
H	4.639798	1.039946	-4.463757
H	4.064477	-1.261844	-2.620984
H	4.867664	0.182114	-1.965343
H	3.424421	-0.464880	-1.182416
H	1.348366	5.320090	0.051760
H	-0.261086	5.696086	0.684122
H	1.066507	6.845167	0.902144
H	-0.685555	5.651108	3.259027
H	0.528309	6.936250	3.265263
H	0.713240	5.557371	4.348986
H	2.876034	6.506637	2.494014
H	3.072708	5.009219	3.417015
H	3.325805	4.995153	1.680183
H	-1.439797	2.665911	4.147748
H	-0.534270	3.963457	4.944414
H	-0.529684	2.336349	5.621989
H	2.067835	3.868252	4.982491
H	2.011380	2.222382	5.616459
H	2.919905	2.560700	4.129932
H	0.682646	0.457128	4.608026
H	1.559700	0.652027	3.072983
H	-0.209220	0.671884	3.095203
H	0.773228	-1.408742	2.895359
H	0.375717	-2.736265	3.982751
H	-2.028400	-1.808869	4.071862
H	-4.399107	-3.186872	0.758828
H	-3.313469	-3.843415	-1.269233
H	-1.764848	-4.630653	-0.935614
H	2.812269	-5.890537	0.751645
H	2.268433	-7.138460	1.885770
H	3.383680	-5.887984	2.433589
H	1.663104	-5.165346	4.363961
H	0.769230	-6.579944	3.801072

H	-0.044944	-5.016966	3.913609
H	-0.824846	-5.225564	1.540041
H	-0.022422	-6.797575	1.463001
H	0.333391	-5.579760	0.233114
H	2.997738	-0.833933	1.755947
H	4.404634	-1.013419	2.786182
H	2.805415	-0.988066	3.517025
H	4.458239	-4.346678	1.303427
H	5.385429	-2.943249	1.850597
H	4.218110	-2.783746	0.524705
H	2.909176	-3.202729	4.654169
H	4.621448	-3.044220	4.249397
H	3.778455	-4.552511	3.895613
H	-0.464483	-1.775612	-4.792079
H	-0.325751	-3.358349	-5.570585
H	0.698888	-2.967424	-4.179019
H	-0.104940	-5.046772	-2.817316
H	-0.813877	-5.410293	-4.388668
H	-1.829776	-5.477448	-2.948285
H	-3.531489	-3.842064	-3.719940
H	-2.694136	-4.070768	-5.256976
H	-3.051907	-2.439458	-4.694180
H	-1.060090	0.182634	-3.365887
H	-2.712962	0.798815	-3.326644
H	-2.341883	-0.642922	-4.267433
H	-4.258350	-1.905812	-2.897796
H	-4.502318	-0.326264	-2.151250
H	-4.248594	-1.743054	-1.135349
H	-2.289416	-0.597666	0.093351
H	-2.820581	0.788326	-0.863419
H	-1.117104	0.319323	-0.851735
C	-6.546174	-0.226727	2.353593
C	-6.907573	-0.154231	3.709561
C	-6.138261	-0.808907	4.676438
C	-4.996530	-1.533672	4.326138
C	-4.627369	-1.642740	2.975843

C	-5.427688	-0.996675	2.018563
H	-7.759368	0.448053	4.013035
H	-6.424105	-0.736430	5.722525
H	-4.404326	-2.025313	5.093391
H	-5.136755	-1.062823	0.977141
C	-8.403775	2.065067	-0.787926
C	-9.186832	1.545966	0.245898
C	-8.615574	0.799640	1.279267
C	-7.234890	0.546327	1.283898
C	-6.470091	1.065550	0.229998
C	-7.018873	1.835811	-0.805601
H	-8.863769	2.674647	-1.560674
H	-10.257382	1.732859	0.250321
H	-9.243494	0.396263	2.068855
H	-5.404900	0.870675	0.224724
C	-5.553607	3.122570	-4.091781
C	-6.486917	2.626054	-3.176484
C	-6.112658	2.407274	-1.839960
C	-4.797279	2.714718	-1.478299
C	-3.833769	3.191893	-2.382373
C	-4.237559	3.397183	-3.713439
H	-5.855101	3.284831	-5.123143
H	-7.490924	2.378978	-3.509443
H	-4.504656	2.544818	-0.452188
H	-3.533487	3.779872	-4.446894

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I in the quintet state SCF = -4240.81170478

Mo	1.896535	2.172569	0.205006
Mo	0.669371	-2.658461	-0.304446
I	4.459505	1.968502	1.463989
I	2.611006	-3.983182	-1.952454
P	2.718677	2.330165	-2.171972
P	0.858383	3.360690	2.195326
P	1.588033	-3.439062	1.831290
P	-1.220947	-2.497116	-2.024981

N	1.347722	0.285923	0.268363
N	1.043174	-0.859680	0.101145
N	0.125084	3.056683	-0.714563
N	-1.067968	-2.823248	0.931479
C	1.192548	3.099697	-2.956455
C	-0.047642	3.102914	-2.086843
C	-1.301569	3.221322	-2.667337
C	-2.463795	3.379037	-1.882739
C	-2.227292	3.548611	-0.503529
C	-0.985275	3.340854	0.050590
C	-0.882689	3.305123	1.558409
C	4.079098	3.624577	-2.572580
C	4.049841	4.134989	-4.028956
C	3.844010	4.824543	-1.629196
C	5.469054	3.031886	-2.268555
C	3.047355	0.687952	-3.082572
C	1.687100	-0.018322	-3.216510
C	3.657843	0.814915	-4.488628
C	3.962642	-0.167641	-2.179326
C	1.253000	5.229393	2.358660
C	0.873033	5.892662	1.015450
C	0.477666	5.934321	3.484484
C	2.769831	5.407283	2.568929
C	0.690024	2.535935	3.911273
C	-0.568509	2.949070	4.701385
C	1.954078	2.812382	4.747523
C	0.617703	1.021467	3.631384
C	0.358554	-2.470413	2.894108
C	-1.014729	-2.530907	2.278641
C	-2.174170	-2.256910	3.002326
C	-3.438219	-2.368706	2.395635
C	-3.459523	-2.973787	1.125709
C	-2.292277	-3.180494	0.420058
C	-2.278844	-3.674277	-0.985701
C	1.220546	-5.300222	2.181036
C	2.452795	-6.159157	1.830327

C	0.777532	-5.557395	3.633991
C	0.078184	-5.767416	1.248465
C	3.286112	-2.972189	2.585054
C	3.334750	-1.437085	2.707616
C	4.388798	-3.384309	1.585846
C	3.564051	-3.563275	3.979718
C	-1.280849	-3.407226	-3.725108
C	-0.208470	-2.776076	-4.636575
C	-0.902498	-4.888450	-3.493662
C	-2.650232	-3.393226	-4.429545
C	-2.350711	-0.920620	-2.110084
C	-2.019231	-0.078738	-3.356449
C	-3.863454	-1.228879	-2.112259
C	-2.049770	-0.058600	-0.863635
H	1.443800	4.150292	-3.145107
H	0.978042	2.658421	-3.934390
H	-1.375945	3.142768	-3.747404
H	-3.045840	3.776281	0.169725
H	-1.527566	4.074967	1.997728
H	-1.274046	2.336495	1.893624
H	3.096794	4.604432	-4.295288
H	4.256343	3.349142	-4.756329
H	4.826330	4.902160	-4.146013
H	5.738000	2.233678	-2.965330
H	5.531641	2.642227	-1.249306
H	6.222332	3.824145	-2.371170
H	2.856792	5.280950	-1.770255
H	4.595415	5.597633	-1.838758
H	3.940146	4.533774	-0.578924
H	1.114036	-0.003201	-2.287715
H	1.080589	0.422951	-4.014948
H	1.858171	-1.068373	-3.467685
H	3.049111	1.444331	-5.148850
H	3.703420	-0.184745	-4.939692
H	4.676597	1.210518	-4.472128
H	4.137336	-1.135535	-2.663132

H	4.930493	0.305693	-1.992876
H	3.493373	-0.369598	-1.213838
H	1.374945	5.412484	0.170041
H	-0.205644	5.872381	0.827693
H	1.185286	6.944543	1.040848
H	-0.605500	5.793025	3.395138
H	0.671460	7.013885	3.432460
H	0.790267	5.597331	4.476248
H	3.010088	6.478899	2.559247
H	3.113816	4.997756	3.521431
H	3.344935	4.915669	1.779496
H	-1.492634	2.721998	4.159035
H	-0.579183	4.007507	4.966782
H	-0.596936	2.376865	5.638126
H	2.018330	3.856573	5.066967
H	1.923304	2.195744	5.655517
H	2.865998	2.556988	4.198562
H	0.553395	0.482158	4.586231
H	1.505617	0.681002	3.096577
H	-0.258703	0.743383	3.034961
H	0.741919	-1.449908	2.834878
H	0.326233	-2.749390	3.953570
H	-2.083097	-1.884471	4.018964
H	-4.405319	-3.216868	0.653727
H	-3.288649	-3.820438	-1.378014
H	-1.761656	-4.639679	-1.029292
H	2.783690	-5.981318	0.801363
H	2.181761	-7.219890	1.915944
H	3.296047	-5.985695	2.501644
H	1.520769	-5.240946	4.368693
H	0.610178	-6.633667	3.776740
H	-0.166391	-5.049124	3.860522
H	-0.867503	-5.262884	1.457513
H	-0.081337	-6.843911	1.398114
H	0.334125	-5.623401	0.191362
H	3.016298	-0.929781	1.796111

H	4.367297	-1.123999	2.897787
H	2.732182	-1.072124	3.544779
H	4.444134	-4.461704	1.421389
H	5.360095	-3.055668	1.978702
H	4.236066	-2.909593	0.612744
H	2.785075	-3.287904	4.700621
H	4.512447	-3.155232	4.354214
H	3.659782	-4.651737	3.975204
H	-0.379376	-1.710740	-4.812800
H	-0.219641	-3.280269	-5.612595
H	0.788370	-2.901672	-4.205673
H	-0.007144	-5.002946	-2.878070
H	-0.687689	-5.351413	-4.465471
H	-1.723945	-5.455560	-3.042121
H	-3.440521	-3.814241	-3.798402
H	-2.589492	-4.016245	-5.332232
H	-2.959965	-2.395206	-4.747161
H	-0.968487	0.213519	-3.377451
H	-2.616852	0.839240	-3.331185
H	-2.254589	-0.593184	-4.290435
H	-4.176069	-1.858275	-2.946996
H	-4.413407	-0.281620	-2.191084
H	-4.181842	-1.707839	-1.183095
H	-2.228275	-0.596196	0.070169
H	-2.712629	0.813554	-0.880219
H	-1.020691	0.302459	-0.847556
C	-6.582914	-0.299972	2.295755
C	-6.962643	-0.266964	3.648154
C	-6.204209	-0.946526	4.606411
C	-5.055045	-1.657176	4.251035
C	-4.667675	-1.726042	2.903371
C	-5.457380	-1.056729	1.954209
H	-7.821100	0.323173	3.956756
H	-6.504694	-0.905263	5.650124
H	-4.471233	-2.168905	5.011576
H	-5.153001	-1.094302	0.915226

C	-8.413416	2.036981	-0.826880
C	-9.206023	1.499620	0.190121
C	-8.643156	0.740220	1.218567
C	-7.261114	0.495421	1.236397
C	-6.485454	1.038102	0.202289
C	-7.026886	1.816624	-0.830349
H	-8.867114	2.652225	-1.598880
H	-10.277760	1.679784	0.183725
H	-9.278593	0.318390	1.992382
H	-5.418463	0.852439	0.206752
C	-5.536893	3.078491	-4.110327
C	-6.476291	2.587389	-3.198058
C	-6.113546	2.395196	-1.853822
C	-4.808038	2.725706	-1.477788
C	-3.837366	3.199502	-2.379314
C	-4.230032	3.374313	-3.720342
H	-5.826653	3.219222	-5.148323
H	-7.473013	2.320862	-3.537597
H	-4.525858	2.573412	-0.445068
H	-3.521957	3.752282	-4.452493

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H in the closed-shell singlet state SCF = -4471.88459228

Mo	-1.899360	2.348500	-0.561784
Mo	-1.554452	-2.431602	0.612496
I	-4.147753	2.681386	-2.346827
I	-3.683195	-3.247868	2.336685
P	-2.955445	2.931622	1.543386
P	-0.273225	3.045522	-2.374053
P	-2.687950	-3.232494	-1.388830
P	0.323181	-2.474681	2.326329
N	-1.674632	0.521217	-0.200490
N	-1.576376	-0.649212	0.087769
N	-0.137131	2.918071	0.590483
N	0.094434	-3.104393	-0.617828
C	-1.508934	3.620677	2.517067

C	-0.173689	3.241928	1.933955
C	0.962026	3.295170	2.721290
C	2.255924	3.111507	2.182680
C	2.282426	3.011916	0.782212
C	1.125363	2.877692	0.036266
C	1.259108	2.565867	-1.431594
C	-4.160407	4.435136	1.591694
C	-4.268955	5.138035	2.962137
C	-3.619323	5.466506	0.574713
C	-5.564129	3.989374	1.138599
C	-3.624221	1.507744	2.638220
C	-2.403327	0.674992	3.086811
C	-4.370822	1.949595	3.909072
C	-4.556801	0.631930	1.774754
C	-0.072929	4.916552	-2.717571
C	0.211574	5.610670	-1.365469
C	1.077651	5.244939	-3.684917
C	-1.399969	5.478187	-3.268822
C	-0.109171	2.011966	-3.972359
C	-1.047320	2.558061	-5.065046
C	-0.585519	0.596632	-3.587569
C	1.331795	1.917589	-4.512484
C	-1.329612	-2.729505	-2.588475
C	0.024115	-2.979725	-1.983629
C	1.169698	-3.047323	-2.771544
C	2.425331	-3.265367	-2.185818
C	2.449018	-3.555351	-0.814160
C	1.284326	-3.505658	-0.065032
C	1.240765	-3.845225	1.386313
C	-2.744898	-5.163408	-1.494242
C	-4.124209	-5.683889	-1.043468
C	-2.403757	-5.693647	-2.899861
C	-1.705120	-5.742190	-0.505000
C	-4.261110	-2.501533	-2.198398
C	-3.976780	-1.015245	-2.489746
C	-5.413002	-2.549388	-1.171155

C	-4.680763	-3.174467	-3.517389
C	0.200769	-3.267435	4.080131
C	-0.775603	-2.413600	4.917805
C	-0.405670	-4.680922	3.923654
C	1.537698	-3.423063	4.828419
C	1.660151	-1.085641	2.351205
C	1.367050	-0.120414	3.514269
C	3.115792	-1.590238	2.453889
C	1.542482	-0.302006	1.029065
H	-1.580330	4.712532	2.439290
H	-1.560486	3.386235	3.584332
H	0.822593	3.459636	3.783848
H	3.222191	2.940880	0.247212
H	2.187561	2.988463	-1.832245
H	1.323934	1.476125	-1.552345
H	-3.303256	5.496922	3.333450
H	-4.714535	4.506596	3.730716
H	-4.915051	6.019066	2.850626
H	-6.041058	3.335337	1.874252
H	-5.536961	3.472249	0.175874
H	-6.203883	4.875022	1.024836
H	-2.605852	5.808026	0.820367
H	-4.270430	6.351202	0.577698
H	-3.613659	5.066708	-0.442305
H	-1.730533	0.436389	2.263779
H	-1.828493	1.187924	3.866662
H	-2.752670	-0.275991	3.502500
H	-3.768190	2.619155	4.533822
H	-4.597006	1.058307	4.509208
H	-5.321751	2.441247	3.688237
H	-4.910197	-0.217353	2.370821
H	-5.429140	1.188292	1.418856
H	-4.039707	0.226387	0.903134
H	-0.563123	5.395228	-0.622157
H	1.177038	5.320388	-0.940726
H	0.230016	6.696322	-1.525995

H	2.034417	4.829313	-3.349172
H	1.197518	6.334914	-3.743481
H	0.880610	4.885289	-4.698305
H	-1.303896	6.565853	-3.386153
H	-1.664692	5.060454	-4.241802
H	-2.237018	5.278646	-2.594258
H	-0.698897	3.513972	-5.467383
H	-2.070414	2.680415	-4.695865
H	-1.072648	1.844743	-5.899718
H	-1.625475	0.615600	-3.253263
H	-0.511072	-0.060803	-4.464685
H	0.021254	0.153080	-2.789753
H	1.329325	1.289671	-5.413464
H	2.013424	1.447972	-3.795823
H	1.746244	2.888026	-4.793304
H	-1.477877	-1.652347	-2.688092
H	-1.388397	-3.159081	-3.594871
H	1.089254	-2.873778	-3.840245
H	3.383613	-3.818853	-0.330183
H	2.236125	-4.055437	1.785171
H	0.637207	-4.749951	1.516475
H	-4.388570	-5.304436	-0.051014
H	-4.089279	-6.780091	-0.985332
H	-4.921756	-5.422406	-1.741652
H	-3.065433	-5.301162	-3.674693
H	-2.498183	-6.787993	-2.907536
H	-1.371136	-5.455831	-3.179762
H	-0.679797	-5.472113	-0.769214
H	-1.772424	-6.838499	-0.521195
H	-1.905202	-5.422777	0.525607
H	-3.546164	-0.490922	-1.635562
H	-4.917427	-0.508271	-2.730193
H	-3.317046	-0.874813	-3.351476
H	-5.704178	-3.563343	-0.892176
H	-6.292497	-2.057286	-1.606878
H	-5.146551	-2.017900	-0.253777

H	-3.872602	-3.159529	-4.258287
H	-5.524049	-2.617077	-3.946343
H	-5.008428	-4.208555	-3.385471
H	-0.411833	-1.396068	5.079865
H	-0.905576	-2.879764	5.903971
H	-1.757031	-2.358813	4.441359
H	-1.303612	-4.684696	3.301332
H	-0.699163	-5.049624	4.914822
H	0.317711	-5.396816	3.517199
H	2.260117	-4.022252	4.262695
H	1.352814	-3.949200	5.774665
H	2.003720	-2.466888	5.076949
H	0.350910	0.279301	3.460275
H	2.058553	0.723278	3.459030
H	1.506377	-0.587850	4.491326
H	3.297763	-2.238064	3.312414
H	3.779383	-0.720535	2.552843
H	3.419757	-2.125094	1.547819
H	1.638155	-0.947547	0.151791
H	2.351320	0.434987	0.993349
H	0.598035	0.235078	0.951817
C	5.927260	-2.191548	-3.145619
C	6.122697	-2.963553	-4.306623
C	5.114547	-3.791613	-4.797635
C	3.891471	-3.888476	-4.135216
C	3.688476	-3.171041	-2.948323
C	4.704668	-2.328857	-2.472173
H	7.075798	-2.926765	-4.824471
H	5.289824	-4.375128	-5.697344
H	3.108523	-4.541464	-4.510875
H	4.505873	-1.732416	-1.586671
C	8.911289	0.618079	-1.832963
C	8.824824	0.253673	-3.173991
C	7.853714	-0.650798	-3.595683
C	6.962032	-1.230923	-2.676049
C	7.065788	-0.853395	-1.325108

C	8.021389	0.076700	-0.889944
H	9.643170	1.354949	-1.515620
H	9.500099	0.697760	-3.900409
H	7.767885	-0.882764	-4.652329
H	6.413211	-1.309777	-0.586310
C	4.520761	2.582797	5.177972
C	5.668878	2.068670	4.576127
C	5.749862	1.982299	3.174057
C	4.641483	2.392449	2.423754
C	3.451512	2.873119	3.008621
C	3.427810	2.984283	4.414951
H	4.470713	2.656031	6.261226
H	6.487797	1.715912	5.194792
H	4.710617	2.328914	1.345707
H	2.548305	3.368085	4.920788
C	8.241829	1.659584	3.090953
C	6.980273	1.491710	2.493901
C	6.930276	0.905608	1.216675
C	8.092101	0.542163	0.520970
C	9.334961	0.710110	1.153370
C	9.402158	1.255476	2.433426
H	8.320185	2.142256	4.059937
H	5.970273	0.756146	0.731693
H	10.243353	0.406952	0.640698
H	10.367453	1.386702	2.915074

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H in the triplet state SCF = -4471.89486556

Mo	-1.848469	2.448655	-0.557856
Mo	-1.571005	-2.370522	0.590127
I	-4.129821	2.777927	-2.282753
I	-3.633302	-3.338506	2.370095
P	-2.949610	2.928754	1.604704
P	-0.216552	2.950305	-2.348502
P	-2.782659	-3.168799	-1.391979
P	0.374874	-2.507058	2.247628

N	-1.562001	0.589337	-0.297365
N	-1.493112	-0.574940	-0.012235
N	-0.092788	2.982469	0.629927
N	0.027692	-2.998368	-0.697905
C	-1.493174	3.686946	2.534698
C	-0.153504	3.299714	1.968822
C	0.974839	3.311185	2.776685
C	2.265179	3.103013	2.249706
C	2.315954	2.997694	0.851223
C	1.166996	2.881686	0.089274
C	1.311001	2.523053	-1.365219
C	-4.208872	4.377161	1.720609
C	-4.303445	5.047755	3.107419
C	-3.742321	5.446611	0.705593
C	-5.603005	3.874247	1.296950
C	-3.501552	1.459267	2.692233
C	-2.220333	0.690057	3.075621
C	-4.235378	1.824962	3.993685
C	-4.407440	0.562987	1.822587
C	-0.002140	4.819511	-2.744702
C	0.236219	5.564686	-1.410909
C	1.183998	5.120882	-3.677910
C	-1.303585	5.372912	-3.361447
C	0.030682	1.901012	-3.930541
C	-0.872867	2.427491	-5.061763
C	-0.462050	0.493600	-3.548782
C	1.489055	1.793215	-4.418470
C	-1.468657	-2.609217	-2.612473
C	-0.091226	-2.863956	-2.063111
C	1.024115	-2.912483	-2.894819
C	2.303080	-3.129460	-2.363205
C	2.369727	-3.468599	-1.001697
C	1.235610	-3.438100	-0.211274
C	1.243375	-3.834087	1.227097
C	-2.820214	-5.091916	-1.558311
C	-4.180085	-5.647241	-1.091772

C	-2.516584	-5.564047	-2.993810
C	-1.742315	-5.690777	-0.624046
C	-4.387696	-2.416230	-2.110502
C	-4.133933	-0.908285	-2.303823
C	-5.519571	-2.551674	-1.068796
C	-4.820416	-3.014270	-3.460832
C	0.302683	-3.360033	3.976140
C	-0.648620	-2.534085	4.868292
C	-0.304290	-4.769887	3.792420
C	1.659867	-3.539813	4.681849
C	1.719473	-1.126062	2.292150
C	1.472900	-0.199525	3.496345
C	3.172894	-1.648396	2.333846
C	1.577874	-0.294890	1.002551
H	-1.590821	4.771314	2.402909
H	-1.535131	3.504188	3.612867
H	0.825831	3.452444	3.841098
H	3.261685	2.900402	0.332812
H	2.247535	2.925335	-1.767963
H	1.373986	1.429402	-1.436824
H	-3.344757	5.455917	3.445086
H	-4.676716	4.375354	3.880107
H	-5.004558	5.890529	3.042570
H	-6.036034	3.199209	2.041012
H	-5.573885	3.360268	0.332137
H	-6.281560	4.732334	1.199364
H	-2.732794	5.820828	0.920608
H	-4.420371	6.309204	0.753478
H	-3.763263	5.070307	-0.320378
H	-1.566577	0.520288	2.220553
H	-1.649234	1.220743	3.846376
H	-2.494721	-0.291665	3.477071
H	-3.645901	2.497671	4.627664
H	-4.409933	0.904036	4.565524
H	-5.210153	2.284386	3.810493
H	-4.700922	-0.323882	2.394520

H	-5.315363	1.083883	1.504740
H	-3.889319	0.219398	0.925434
H	-0.571397	5.393404	-0.691318
H	1.178527	5.280267	-0.933249
H	0.278083	6.642911	-1.612414
H	2.129354	4.723953	-3.291075
H	1.300895	6.208943	-3.771911
H	1.029844	4.723935	-4.684397
H	-1.196380	6.456262	-3.508162
H	-1.536123	4.928659	-4.330785
H	-2.167468	5.198895	-2.713976
H	-0.517717	3.378344	-5.469266
H	-1.907292	2.552913	-4.724371
H	-0.872962	1.701478	-5.885958
H	-1.514710	0.522670	-3.258960
H	-0.351611	-0.177389	-4.411750
H	0.105206	0.057672	-2.719484
H	1.516621	1.155936	-5.312704
H	2.140237	1.323801	-3.673428
H	1.922857	2.756896	-4.692871
H	-1.637982	-1.533461	-2.668792
H	-1.561328	-3.007383	-3.628831
H	0.899818	-2.712658	-3.954916
H	3.318187	-3.755320	-0.559044
H	2.249723	-4.073734	1.579371
H	0.628164	-4.734424	1.338105
H	-4.428335	-5.302015	-0.082908
H	-4.125974	-6.743828	-1.067497
H	-4.996238	-5.378576	-1.766046
H	-3.204884	-5.149844	-3.734056
H	-2.602773	-6.658074	-3.038686
H	-1.494840	-5.306747	-3.294562
H	-0.730786	-5.387571	-0.905598
H	-1.789739	-6.786416	-0.687901
H	-1.917067	-5.416288	0.422669
H	-3.708399	-0.438135	-1.416140

H	-5.085591	-0.405225	-2.507053
H	-3.479862	-0.691239	-3.153426
H	-5.798061	-3.586004	-0.862173
H	-6.410492	-2.037753	-1.453154
H	-5.242700	-2.086343	-0.119050
H	-4.027499	-2.938598	-4.214140
H	-5.683440	-2.450544	-3.839019
H	-5.123616	-4.061639	-3.383279
H	-0.274103	-1.525426	5.060342
H	-0.759301	-3.036001	5.839057
H	-1.640375	-2.456557	4.416790
H	-1.221152	-4.757223	3.199675
H	-0.562734	-5.172512	4.780203
H	0.408360	-5.467261	3.337941
H	2.364556	-4.123759	4.078996
H	1.498698	-4.094274	5.616190
H	2.135466	-2.592985	4.946992
H	0.456709	0.202892	3.492977
H	2.165521	0.643846	3.446524
H	1.644115	-0.699339	4.451924
H	3.372431	-2.334431	3.157665
H	3.847272	-0.789493	2.453299
H	3.446387	-2.145789	1.397453
H	1.623013	-0.911168	0.101542
H	2.406146	0.420538	0.963088
H	0.646599	0.269032	0.977025
C	5.798968	-2.018328	-3.292121
C	5.963016	-2.680947	-4.523778
C	4.931290	-3.441089	-5.073023
C	3.718341	-3.584665	-4.400688
C	3.544419	-2.979388	-3.147987
C	4.582551	-2.196245	-2.618302
H	6.908460	-2.615559	-5.052530
H	5.082493	-3.939486	-6.026778
H	2.921324	-4.191956	-4.820896
H	4.404648	-1.679301	-1.680190

C	8.870953	0.574254	-1.745384
C	8.790134	0.308908	-3.109767
C	7.789284	-0.521777	-3.606822
C	6.860707	-1.130427	-2.743621
C	6.958792	-0.851474	-1.367624
C	7.943270	0.006441	-0.855985
H	9.627846	1.254820	-1.366617
H	9.494454	0.773750	-3.794430
H	7.712394	-0.673955	-4.678382
H	6.277771	-1.330117	-0.669853
C	4.494714	2.502884	5.259874
C	5.616444	1.928469	4.663267
C	5.704519	1.834866	3.262356
C	4.617111	2.295209	2.509705
C	3.451618	2.832471	3.089045
C	3.425161	2.956341	4.491486
H	4.446126	2.582647	6.342514
H	6.411989	1.538081	5.289552
H	4.682915	2.220569	1.433114
H	2.564182	3.387984	4.990680
C	8.172062	1.349502	3.211275
C	6.915126	1.291116	2.584373
C	6.857013	0.771784	1.278071
C	8.009359	0.377065	0.583691
C	9.246096	0.434519	1.246623
C	9.318807	0.906203	2.555244
H	8.263063	1.778641	4.203860
H	5.902589	0.703337	0.764975
H	10.145319	0.106511	0.733181
H	10.279548	0.952095	3.060942

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H in the quintet state SCF = -4471.88668785

Mo	-1.691686	2.497664	-0.524769
Mo	-1.706618	-2.387010	0.568300
I	-3.900914	2.781074	-2.318278

I	-3.828648	-3.180482	2.358366
P	-2.851792	3.057791	1.651170
P	-0.003003	3.031464	-2.347830
P	-2.897306	-3.128568	-1.439417
P	0.231469	-2.526521	2.226432
N	-1.654259	0.562581	-0.340266
N	-1.638867	-0.592180	-0.031864
N	0.043183	3.102311	0.649815
N	-0.086113	-2.984456	-0.722616
C	-1.376001	3.768131	2.563144
C	-0.035659	3.339421	2.016682
C	1.066241	3.272499	2.844610
C	2.370734	3.032525	2.342971
C	2.445192	2.990623	0.931046
C	1.321344	2.967974	0.139856
C	1.488693	2.629169	-1.322965
C	-4.073088	4.533899	1.672765
C	-4.175261	5.232916	3.045229
C	-3.561642	5.565166	0.641106
C	-5.470996	4.054250	1.234659
C	-3.482401	1.609727	2.715535
C	-2.237856	0.774843	3.079940
C	-4.192359	2.008606	4.020189
C	-4.431460	0.759455	1.843467
C	0.201268	4.884695	-2.791527
C	0.470929	5.651743	-1.476739
C	1.369953	5.156368	-3.755608
C	-1.117236	5.418680	-3.387226
C	0.218685	1.920038	-3.885161
C	-0.655881	2.431845	-5.046294
C	-0.306678	0.531993	-3.471752
C	1.683014	1.778966	-4.347448
C	-1.564664	-2.552209	-2.639211
C	-0.194170	-2.830877	-2.085747
C	0.925686	-2.886159	-2.911419
C	2.198096	-3.125905	-2.374486

C	2.252247	-3.477540	-1.015775
C	1.112705	-3.441964	-0.232570
C	1.104487	-3.851594	1.201354
C	-2.938254	-5.048098	-1.625770
C	-4.307193	-5.599286	-1.182265
C	-2.611368	-5.513747	-3.057531
C	-1.879543	-5.653326	-0.673500
C	-4.488493	-2.363339	-2.178741
C	-4.227771	-0.853398	-2.342755
C	-5.639860	-2.509258	-1.160178
C	-4.896027	-2.941933	-3.545221
C	0.139657	-3.400814	3.942412
C	-0.780219	-2.561282	4.854773
C	-0.516832	-4.785842	3.740776
C	1.496042	-3.632993	4.634328
C	1.586605	-1.157946	2.293419
C	1.364377	-0.258871	3.521604
C	3.036346	-1.691981	2.310254
C	1.434873	-0.294909	1.024696
H	-1.445115	4.854814	2.426867
H	-1.438472	3.584818	3.640018
H	0.899617	3.397600	3.908977
H	3.397481	2.869104	0.429131
H	2.415782	3.061924	-1.714517
H	1.586669	1.537729	-1.399978
H	-3.214288	5.632713	3.386015
H	-4.568739	4.580881	3.825598
H	-4.861711	6.084555	2.952484
H	-5.935637	3.409713	1.986177
H	-5.438377	3.517135	0.282267
H	-6.122475	4.928162	1.103792
H	-2.548964	5.921136	0.866791
H	-4.225002	6.440304	0.655664
H	-3.564480	5.158282	-0.373187
H	-1.610060	0.569838	2.212145
H	-1.626799	1.273043	3.841087

H	-2.558317	-0.192681	3.481434
H	-3.572941	2.658308	4.649989
H	-4.402915	1.097549	4.595048
H	-5.148466	2.507517	3.839649
H	-4.736490	-0.129311	2.405993
H	-5.333280	1.308011	1.557039
H	-3.941420	0.412614	0.931394
H	-0.315376	5.480062	-0.734572
H	1.429406	5.381940	-1.022585
H	0.498210	6.726251	-1.698360
H	2.322421	4.776133	-3.368979
H	1.481724	6.240898	-3.885954
H	1.202988	4.726521	-4.746534
H	-1.017788	6.498225	-3.562640
H	-1.373920	4.950161	-4.339419
H	-1.958706	5.255836	-2.707715
H	-0.284898	3.370665	-5.466417
H	-1.696597	2.571894	-4.736971
H	-0.642998	1.687043	-5.852885
H	-1.366349	0.581741	-3.210088
H	-0.183311	-0.163465	-4.312852
H	0.230435	0.110328	-2.616003
H	1.712846	1.121568	-5.226306
H	2.315921	1.316847	-3.582731
H	2.133860	2.730703	-4.636173
H	-1.723920	-1.473123	-2.671917
H	-1.653903	-2.927171	-3.664981
H	0.811006	-2.675093	-3.970367
H	3.194012	-3.780382	-0.569750
H	2.106302	-4.098045	1.561158
H	0.485422	-4.750785	1.299356
H	-4.568840	-5.255509	-0.175872
H	-4.259895	-6.696257	-1.160702
H	-5.111692	-5.323324	-1.867405
H	-3.291686	-5.099206	-3.805026
H	-2.690267	-6.608087	-3.109429

H	-1.587236	-5.247862	-3.342347
H	-0.861254	-5.359523	-0.939520
H	-1.934865	-6.748891	-0.732229
H	-2.068696	-5.374742	0.370657
H	-3.834784	-0.397823	-1.432797
H	-5.171773	-0.347748	-2.575266
H	-3.541715	-0.621156	-3.162703
H	-5.933830	-3.544526	-0.981966
H	-6.518879	-1.977196	-1.547694
H	-5.372963	-2.069107	-0.195437
H	-4.088854	-2.857970	-4.282489
H	-5.751376	-2.372710	-3.932867
H	-5.201941	-3.989993	-3.487440
H	-0.368880	-1.572351	5.070484
H	-0.908288	-3.081554	5.813712
H	-1.769178	-2.437639	4.407032
H	-1.444086	-4.729646	3.165933
H	-0.770778	-5.200752	4.724710
H	0.162631	-5.497826	3.259079
H	2.177632	-4.229525	4.017310
H	1.326728	-4.194620	5.563031
H	2.001983	-2.703996	4.906342
H	0.346435	0.136006	3.554094
H	2.048638	0.590075	3.469164
H	1.566212	-0.776904	4.461470
H	3.233978	-2.402325	3.114410
H	3.717822	-0.842228	2.450270
H	3.300553	-2.165802	1.359153
H	1.453349	-0.891762	0.109579
H	2.271264	0.410613	0.987352
H	0.511035	0.282696	1.027561
C	5.723747	-2.088775	-3.284118
C	5.870028	-2.734311	-4.526983
C	4.818885	-3.458117	-5.088328
C	3.603065	-3.581795	-4.417402
C	3.444462	-2.992472	-3.154899

C	4.502500	-2.245030	-2.612990
H	6.817119	-2.684913	-5.054519
H	4.957012	-3.944654	-6.050186
H	2.791154	-4.162548	-4.846567
H	4.339116	-1.739898	-1.665801
C	8.874523	0.376759	-1.688409
C	8.783180	0.144658	-3.058348
C	7.756563	-0.643725	-3.571830
C	6.811361	-1.242843	-2.719975
C	6.920120	-0.997356	-1.338661
C	7.931153	-0.181556	-0.809796
H	9.653223	1.024036	-1.295625
H	9.500579	0.602591	-3.734098
H	7.673696	-0.770036	-4.646381
H	6.226142	-1.470296	-0.649900
C	4.477764	2.120369	5.358256
C	5.603539	1.559161	4.753298
C	5.729252	1.578359	3.351649
C	4.689576	2.142015	2.604917
C	3.512343	2.661233	3.186678
C	3.447265	2.665313	4.598022
H	4.393342	2.112887	6.441887
H	6.366158	1.089345	5.366142
H	4.801471	2.164443	1.529492
H	2.578664	3.070714	5.106368
C	8.185384	1.030828	3.298234
C	6.931533	1.032144	2.663275
C	6.864452	0.559051	1.340327
C	8.007330	0.151494	0.638273
C	9.242640	0.153206	1.306362
C	9.322459	0.578545	2.630789
H	8.279454	1.420094	4.307156
H	5.908766	0.536710	0.825096
H	10.134361	-0.184708	0.786094
H	10.281960	0.579263	3.141096

III in the triplet state SCF = -4240.75738213

Mo	-9.435567	-0.584392	0.601845
Mo	9.473598	-0.160782	0.278209
I	-11.353202	-2.211790	1.923017
I	11.965230	-0.106776	1.662926
P	-9.716875	1.567154	1.875870
P	-8.565860	-2.221797	-1.100436
P	8.769500	2.072776	0.956747
P	9.258763	-2.572636	-0.172353
N	9.927597	0.860041	-2.601978
N	9.762302	0.481075	-1.536215
N	-7.981927	0.643022	-0.402434
N	7.296119	-0.289174	-0.087616
C	-9.091012	2.673751	0.495108
C	-7.989029	2.034629	-0.311271
C	-7.048112	2.830114	-0.928353
C	-6.007972	2.292666	-1.721110
C	-6.018938	0.882242	-1.824026
C	-6.960524	0.105329	-1.184255
C	-6.892238	-1.396497	-1.302499
C	-11.453957	2.272078	2.221905
C	-11.511589	3.811750	2.262572
C	-12.356008	1.773147	1.068281
C	-11.994920	1.683730	3.540024
C	-8.519873	1.809975	3.339170
C	-7.085074	1.650169	2.787284
C	-8.634843	3.183799	4.020214
C	-8.773867	0.684811	4.365277
C	-9.405005	-2.140198	-2.809850
C	-9.293410	-0.680225	-3.305476
C	-8.771256	-3.065363	-3.862112
C	-10.900618	-2.479268	-2.633614
C	-8.094478	-4.001780	-0.601071
C	-6.926940	-4.593020	-1.416115
C	-9.331892	-4.914825	-0.707677

C	-7.674424	-3.932245	0.885952
C	7.288861	2.174865	-0.207083
C	6.565186	0.857872	-0.275480
C	5.197090	0.821979	-0.520878
C	4.510557	-0.398071	-0.597982
C	5.270660	-1.558405	-0.400190
C	6.634643	-1.486303	-0.138205
C	7.406257	-2.748560	0.143700
C	7.967251	2.063821	2.714347
C	8.969782	2.577236	3.765936
C	6.650373	2.856766	2.803178
C	7.663840	0.586413	3.063663
C	9.633571	3.761510	0.645982
C	9.942371	3.848708	-0.865386
C	10.991050	3.783640	1.380685
C	8.787750	4.982643	1.047781
C	9.920745	-3.901711	1.051148
C	11.419606	-4.119714	0.769030
C	9.772734	-3.302385	2.469195
C	9.177989	-5.253296	1.036322
C	9.444419	-3.169085	-1.989700
C	10.846016	-2.746218	-2.477171
C	9.257574	-4.677884	-2.223246
C	8.376756	-2.425895	-2.825024
H	-9.972057	2.824004	-0.143339
H	-8.788183	3.664460	0.850762
H	-7.105521	3.901900	-0.764991
H	-5.283961	0.378679	-2.444699
H	-6.384089	-1.691428	-2.227019
H	-6.297553	-1.800938	-0.472532
H	-11.189254	4.262480	1.318006
H	-10.908226	4.237765	3.066422
H	-12.550620	4.123768	2.431049
H	-11.474781	2.084135	4.415710
H	-11.922083	0.591022	3.552462
H	-13.054944	1.949499	3.641886

H	-12.012324	2.119768	0.086251
H	-13.369933	2.167847	1.214190
H	-12.419245	0.680903	1.047086
H	-6.951113	0.696243	2.266478
H	-6.812176	2.450766	2.093404
H	-6.379491	1.679944	3.627442
H	-8.505178	4.008152	3.309950
H	-7.846502	3.277025	4.778712
H	-9.593220	3.313181	4.530085
H	-8.027868	0.754559	5.167975
H	-9.763214	0.750350	4.823833
H	-8.689277	-0.305249	3.904398
H	-9.705271	0.030320	-2.581215
H	-8.259783	-0.386158	-3.510994
H	-9.862026	-0.581222	-4.238944
H	-7.697834	-2.878917	-3.980594
H	-9.245571	-2.882384	-4.835211
H	-8.914722	-4.122776	-3.624201
H	-11.415286	-2.348701	-3.594791
H	-11.063319	-3.509072	-2.307307
H	-11.377724	-1.821651	-1.898840
H	-6.010334	-4.002784	-1.312611
H	-7.154652	-4.684241	-2.479878
H	-6.706444	-5.600662	-1.039991
H	-9.621896	-5.096584	-1.746905
H	-9.095464	-5.889027	-0.260708
H	-10.189615	-4.499702	-0.167704
H	-7.376258	-4.935033	1.219035
H	-8.497201	-3.595217	1.523566
H	-6.816322	-3.268872	1.048563
H	7.738752	2.367487	-1.187167
H	6.585490	2.989666	-0.007024
H	4.659816	1.757838	-0.631752
H	4.801507	-2.534331	-0.467760
H	6.951610	-3.598113	-0.377384
H	7.317269	-2.961809	1.215660

H	9.929608	2.053719	3.696214
H	8.561299	2.396514	4.769234
H	9.150533	3.651425	3.679567
H	6.770375	3.907597	2.528925
H	6.275143	2.825787	3.835174
H	5.873210	2.422944	2.164118
H	6.912612	0.144806	2.403606
H	7.273627	0.530567	4.089132
H	8.572231	-0.032101	3.035410
H	10.509292	2.983973	-1.216414
H	10.552599	4.743129	-1.045373
H	9.042721	3.948046	-1.481257
H	10.890650	3.790644	2.466643
H	11.530553	4.697299	1.096459
H	11.607858	2.922923	1.108604
H	7.811089	4.990672	0.550052
H	9.312888	5.900363	0.750322
H	8.623583	5.039968	2.127145
H	11.585230	-4.628812	-0.185612
H	11.850895	-4.752673	1.556005
H	11.967797	-3.172151	0.764487
H	10.336531	-2.374260	2.581677
H	10.164535	-4.019878	3.202218
H	8.725851	-3.112150	2.739026
H	8.105197	-5.142539	1.229312
H	9.583577	-5.887000	1.836464
H	9.299513	-5.799327	0.101068
H	11.003258	-1.671054	-2.368455
H	10.953174	-3.000598	-3.540257
H	11.643235	-3.258367	-1.930692
H	10.058859	-5.269695	-1.772913
H	9.276062	-4.877010	-3.303363
H	8.298070	-5.044006	-1.841145
H	7.362204	-2.770168	-2.594915
H	8.556123	-2.628105	-3.888953
H	8.410975	-1.344197	-2.686479

C	1.081560	0.410039	-2.022184
C	0.300308	-0.560985	-1.372807
C	0.882886	-1.465542	-0.486349
C	2.252509	-1.423412	-0.234109
C	3.057632	-0.460092	-0.865610
C	2.456406	0.447251	-1.751097
H	-0.763213	-0.619233	-1.585273
H	0.265765	-2.209979	0.009203
H	2.694716	-2.115990	0.476081
H	3.070540	1.193634	-2.246116
C	-4.286889	5.264121	-3.315985
C	-3.029044	4.740024	-3.616364
C	-2.734809	3.401619	-3.302135
C	-3.721094	2.621758	-2.686497
C	-4.997393	3.130759	-2.371180
C	-5.259463	4.477697	-2.706324
H	-4.511532	6.298546	-3.563580
H	-2.267822	5.371206	-4.065039
H	-3.486585	1.591461	-2.437961
H	-6.242189	4.899126	-2.517630
C	-0.714371	3.163552	-4.782850
C	-1.399923	2.824292	-3.604215
C	-0.788074	1.927533	-2.715612
C	0.468348	1.364111	-2.980402
C	1.130393	1.722749	-4.165835
C	0.539441	2.618592	-5.055710
H	-1.179391	3.836506	-5.497330
H	-1.280503	1.699322	-1.774969
H	2.092691	1.277550	-4.402384
H	1.051110	2.878258	-5.978609

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III in the quintet state SCF = -4240.77203208

Mo	-9.437598	-0.569165	0.603232
Mo	9.457036	-0.148349	0.367920
I	-11.351893	-2.152889	1.984275

I	12.090017	-0.100593	1.372643
P	-9.709736	1.618911	1.812483
P	-8.564891	-2.262711	-1.040211
P	8.719945	2.128169	1.051344
P	9.219927	-2.593670	-0.124071
N	9.930895	0.697671	-2.549606
N	9.745545	0.361122	-1.473141
N	-7.989856	0.627950	-0.445546
N	7.297010	-0.272608	0.000045
C	-9.096199	2.684497	0.394552
C	-7.999803	2.021568	-0.399905
C	-7.063326	2.798491	-1.047330
C	-6.024200	2.237079	-1.823697
C	-6.030653	0.824401	-1.878944
C	-6.968982	0.066826	-1.211200
C	-6.895656	-1.438067	-1.279090
C	-11.442167	2.338114	2.153653
C	-11.497703	3.878509	2.147152
C	-12.355961	1.805134	1.024774
C	-11.971052	1.791868	3.494453
C	-8.498447	1.903535	3.256567
C	-7.068529	1.725450	2.697513
C	-8.605496	3.296883	3.898256
C	-8.744116	0.809200	4.317504
C	-9.405962	-2.253027	-2.750145
C	-9.306596	-0.811114	-3.299323
C	-8.762731	-3.211295	-3.766318
C	-10.899326	-2.597806	-2.564513
C	-8.084307	-4.019309	-0.471617
C	-6.915273	-4.640188	-1.262337
C	-9.319328	-4.938842	-0.540126
C	-7.664249	-3.889364	1.011270
C	7.283226	2.182163	-0.151471
C	6.551000	0.868419	-0.190894
C	5.184833	0.832695	-0.431036
C	4.489974	-0.384447	-0.504605

C	5.258575	-1.539180	-0.300908
C	6.621226	-1.466561	-0.047831
C	7.389909	-2.726307	0.252971
C	7.889938	2.193533	2.787698
C	8.871650	2.730785	3.846231
C	6.587604	3.016095	2.808658
C	7.546911	0.735422	3.175250
C	9.647500	3.763001	0.679753
C	9.996831	3.760733	-0.825638
C	10.982266	3.794570	1.454129
C	8.817936	5.020099	0.997836
C	9.930968	-3.880131	1.111364
C	11.408032	-4.149824	0.764800
C	9.868808	-3.232186	2.514224
C	9.154021	-5.211731	1.170716
C	9.376607	-3.209341	-1.928250
C	10.777671	-2.818036	-2.443548
C	9.157821	-4.718623	-2.132506
C	8.303306	-2.457772	-2.749232
H	-9.982373	2.815460	-0.240998
H	-8.790755	3.685406	0.718229
H	-7.121821	3.875109	-0.919632
H	-5.294353	0.302899	-2.483056
H	-6.390551	-1.761252	-2.195975
H	-6.294005	-1.812028	-0.439919
H	-11.184811	4.299604	1.185818
H	-10.885707	4.328519	2.931198
H	-12.534637	4.196997	2.316670
H	-11.441586	2.218406	4.351998
H	-11.899393	0.699973	3.540116
H	-13.029678	2.062407	3.598344
H	-12.020673	2.120269	0.029341
H	-13.367868	2.206180	1.167614
H	-12.421094	0.712859	1.038177
H	-6.939556	0.755653	2.205593
H	-6.800846	2.503832	1.976911

H	-6.355816	1.780740	3.530359
H	-8.483141	4.099706	3.162627
H	-7.808949	3.412044	4.645056
H	-9.558261	3.442124	4.414470
H	-7.990671	0.901224	5.110980
H	-9.729120	0.889371	4.782981
H	-8.664865	-0.193939	3.884741
H	-9.729122	-0.078870	-2.603281
H	-8.275131	-0.513824	-3.511353
H	-9.871873	-0.752530	-4.238234
H	-7.690175	-3.022194	-3.887950
H	-9.235123	-3.067690	-4.746908
H	-8.899921	-4.259973	-3.489361
H	-11.413624	-2.498373	-3.529646
H	-11.055840	-3.619131	-2.209582
H	-11.382223	-1.922821	-1.849645
H	-6.002224	-4.039778	-1.189934
H	-7.145630	-4.783142	-2.319888
H	-6.686899	-5.627568	-0.840049
H	-9.609655	-5.161896	-1.571096
H	-9.080873	-5.894025	-0.054893
H	-10.177015	-4.503552	-0.016296
H	-7.362986	-4.877203	1.383886
H	-8.488746	-3.530494	1.634435
H	-6.808303	-3.217474	1.148111
H	7.755432	2.340870	-1.126874
H	6.588442	3.010374	0.017066
H	4.653479	1.771543	-0.550800
H	4.792967	-2.518218	-0.355794
H	6.922461	-3.589398	-0.232460
H	7.333271	-2.908640	1.333356
H	9.824231	2.189839	3.828719
H	8.431305	2.596767	4.843076
H	9.075148	3.797461	3.723171
H	6.736293	4.050451	2.488581
H	6.190547	3.040788	3.832189

H	5.817197	2.566800	2.172952
H	6.832163	0.277905	2.486411
H	7.095869	0.727696	4.176937
H	8.445288	0.105646	3.219706
H	10.533089	2.856301	-1.121662
H	10.648612	4.619212	-1.031571
H	9.116287	3.867416	-1.466833
H	10.849745	3.847750	2.535597
H	11.542037	4.688815	1.149717
H	11.596509	2.918245	1.230700
H	7.856512	5.025200	0.471684
H	9.373439	5.909137	0.671221
H	8.625559	5.133416	2.068332
H	11.512868	-4.713181	-0.167342
H	11.863062	-4.751028	1.562885
H	11.979003	-3.219699	0.680702
H	10.491298	-2.336965	2.578595
H	10.241604	-3.951567	3.255084
H	8.846393	-2.967114	2.812129
H	8.102982	-5.069227	1.444521
H	9.604002	-5.846547	1.945464
H	9.189295	-5.769980	0.235033
H	10.962687	-1.746988	-2.343916
H	10.855545	-3.077980	-3.507674
H	11.573796	-3.348931	-1.914095
H	9.950361	-5.319490	-1.678623
H	9.162888	-4.935345	-3.209087
H	8.193840	-5.058248	-1.736792
H	7.289585	-2.788557	-2.497408
H	8.462659	-2.670013	-3.814185
H	8.352911	-1.376200	-2.618118
C	1.073722	0.386893	-1.978145
C	0.287374	-0.577003	-1.324294
C	0.864563	-1.463874	-0.416375
C	2.230329	-1.409540	-0.146883
C	3.041389	-0.451690	-0.781118

C	2.444165	0.438117	-1.688119
H	-0.772302	-0.646354	-1.552259
H	0.245560	-2.204843	0.082475
H	2.667264	-2.089696	0.578698
H	3.061283	1.178732	-2.188465
C	-4.312671	5.154867	-3.523490
C	-3.046466	4.630673	-3.785722
C	-2.743486	3.308879	-3.414403
C	-3.731227	2.545471	-2.780365
C	-5.014777	3.056107	-2.500522
C	-5.285773	4.385095	-2.893502
H	-4.543138	6.176072	-3.816488
H	-2.285180	5.250663	-4.249605
H	-3.491772	1.528268	-2.486743
H	-6.274681	4.803873	-2.733177
C	-0.697291	3.039370	-4.853315
C	-1.398931	2.733564	-3.674967
C	-0.794263	1.872614	-2.746769
C	0.470779	1.311115	-2.971696
C	1.149219	1.637272	-4.157367
C	0.565844	2.497560	-5.086404
H	-1.156256	3.682551	-5.598537
H	-1.300363	1.670151	-1.807466
H	2.118911	1.192802	-4.362889
H	1.090812	2.730688	-6.008999

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IV in the triplet state SCF = -4471.82044248

Mo	10.972580	-0.417871	0.308209
Mo	-10.543632	0.078494	0.557615
I	13.306451	-2.022097	0.548513
I	-13.040250	1.348362	1.086029
P	11.479508	0.820674	-1.820358
P	9.721094	-1.145532	2.367082
P	-9.243775	2.126018	0.372504
P	-11.321992	-2.181386	-0.030515

N	-9.221259	-0.528998	3.282690
N	-9.711379	-0.307159	2.274314
N	9.203457	0.794415	0.133825
N	-8.751525	-0.678363	-0.501886
C	10.408487	2.309119	-1.415540
C	9.155287	1.935718	-0.665025
C	8.025843	2.717600	-0.785069
C	6.828309	2.420169	-0.095706
C	6.887094	1.264591	0.715953
C	8.025044	0.493259	0.813543
C	8.021643	-0.738523	1.681284
C	13.194373	1.606284	-2.108109
C	13.163667	2.891184	-2.958476
C	13.748677	1.954355	-0.706641
C	14.130392	0.561478	-2.745457
C	10.751302	0.051577	-3.406841
C	9.226486	-0.084538	-3.193206
C	10.993860	0.884210	-4.676812
C	11.345733	-1.363047	-3.576130
C	9.961867	-0.039943	3.900454
C	9.616757	1.408355	3.484037
C	9.077435	-0.427780	5.097771
C	11.452058	-0.084653	4.302818
C	9.549838	-2.992369	2.819192
C	8.221511	-3.346047	3.516703
C	10.741851	-3.421983	3.695775
C	9.629109	-3.770002	1.484594
C	-7.549934	1.298622	0.360341
C	-7.572576	0.022206	-0.435660
C	-6.420997	-0.421341	-1.075021
C	-6.410426	-1.625850	-1.793254
C	-7.621087	-2.330102	-1.846526
C	-8.764925	-1.840052	-1.224641
C	-10.072028	-2.569399	-1.391388
C	-9.397663	2.881326	-1.399508
C	-10.390376	4.059996	-1.395819

C	-8.054254	3.312524	-2.014386
C	-10.010646	1.783267	-2.302993
C	-8.982051	3.532741	1.657324
C	-8.501128	2.874749	2.970342
C	-10.339509	4.201054	1.961849
C	-7.947978	4.589511	1.231128
C	-12.956349	-2.457693	-1.006869
C	-14.127586	-2.475011	-0.005137
C	-13.124456	-1.229759	-1.932148
C	-13.003081	-3.720286	-1.892192
C	-11.044622	-3.598297	1.235128
C	-11.762389	-3.202276	2.542472
C	-11.520324	-4.991285	0.790709
C	-9.524577	-3.677591	1.502405
H	11.052351	2.926509	-0.774681
H	10.168532	2.913462	-2.296982
H	8.064728	3.567521	-1.459898
H	6.026642	0.978633	1.313221
H	7.252332	-0.665659	2.457557
H	7.772961	-1.616437	1.069655
H	12.544074	3.671271	-2.503163
H	12.803625	2.719332	-3.974603
H	14.183230	3.290941	-3.035013
H	13.855330	0.337659	-3.780482
H	14.139434	-0.370865	-2.170431
H	15.154100	0.957340	-2.758081
H	13.113058	2.667279	-0.167577
H	14.735228	2.422306	-0.821036
H	13.869625	1.061070	-0.086862
H	8.988697	-0.646300	-2.284073
H	8.726690	0.886283	-3.126322
H	8.798513	-0.624047	-4.047880
H	10.620662	1.909314	-4.573885
H	10.458475	0.423066	-5.517245
H	12.051904	0.925946	-4.948639
H	10.870768	-1.852470	-4.436846

H	12.423543	-1.349038	-3.754905
H	11.166633	-1.981550	-2.689843
H	10.205836	1.738671	2.622178
H	8.558982	1.530842	3.233010
H	9.841031	2.077900	4.324328
H	8.013603	-0.445411	4.835050
H	9.205684	0.315356	5.895724
H	9.347841	-1.401715	5.514524
H	11.626846	0.633068	5.115298
H	11.763532	-1.069457	4.658880
H	12.103111	0.183839	3.463783
H	7.352737	-3.107916	2.893994
H	8.099688	-2.843929	4.478499
H	8.197292	-4.427244	3.705855
H	10.689005	-2.992871	4.700680
H	10.729036	-4.513907	3.806428
H	11.698670	-3.143977	3.241335
H	9.514458	-4.842471	1.690163
H	10.591918	-3.622957	0.986543
H	8.831592	-3.487625	0.786771
H	-7.378881	1.038241	1.410860
H	-6.716168	1.933742	0.044222
H	-5.527079	0.190620	-1.022616
H	-7.678265	-3.280098	-2.367184
H	-9.897335	-3.641183	-1.534791
H	-10.535241	-2.207310	-2.317280
H	-11.342134	3.779836	-0.930714
H	-10.598187	4.357306	-2.432488
H	-9.995384	4.939092	-0.880907
H	-7.535704	4.062643	-1.412697
H	-8.230282	3.749062	-3.006854
H	-7.381290	2.458551	-2.150542
H	-9.356128	0.914635	-2.414647
H	-10.182741	2.195211	-3.306912
H	-10.989138	1.450448	-1.927714
H	-9.167088	2.072879	3.296501

H	-8.488235	3.638176	3.758860
H	-7.484449	2.474971	2.898756
H	-10.745102	4.753035	1.113075
H	-10.204162	4.917041	2.783746
H	-11.087435	3.464843	2.268065
H	-6.973578	4.145104	0.996750
H	-7.792910	5.297344	2.056734
H	-8.276660	5.170356	0.365561
H	-14.124751	-3.379632	0.611339
H	-15.077950	-2.458183	-0.555183
H	-14.106615	-1.599707	0.651789
H	-13.189747	-0.297883	-1.366418
H	-14.056727	-1.337323	-2.502318
H	-12.312085	-1.139706	-2.665050
H	-12.189363	-3.747181	-2.625228
H	-13.943940	-3.718053	-2.458745
H	-12.974658	-4.647744	-1.320073
H	-11.417668	-2.235218	2.915558
H	-11.556385	-3.957747	3.312678
H	-12.847052	-3.143862	2.415195
H	-12.607746	-5.046568	0.698213
H	-11.220219	-5.729974	1.546198
H	-11.073570	-5.299358	-0.161505
H	-8.972636	-4.049785	0.632037
H	-9.345326	-4.379946	2.326800
H	-9.099665	-2.715750	1.792757
C	-2.746986	-2.320625	-2.527326
C	-2.856371	-3.054812	-3.719923
C	-4.107110	-3.316254	-4.278060
C	-5.267120	-2.852455	-3.661160
C	-5.188780	-2.119074	-2.464508
C	-3.922672	-1.866608	-1.913969
H	-1.955901	-3.395567	-4.222546
H	-4.177091	-3.868764	-5.210954
H	-6.232728	-3.032326	-4.124163
H	-3.848612	-1.348408	-0.962750

C	1.084605	-1.436513	-0.806008
C	0.840856	-2.693026	-1.358387
C	-0.401502	-2.991274	-1.916436
C	-1.421664	-2.026650	-1.926956
C	-1.160119	-0.766110	-1.370975
C	0.084027	-0.450213	-0.806223
H	2.047781	-1.221412	-0.352290
H	1.619367	-3.450979	-1.339210
H	-0.592685	-3.980749	-2.322004
H	-1.924327	0.003715	-1.425949
C	4.531281	5.385171	-0.614079
C	3.274868	4.811433	-0.414131
C	3.169927	3.442066	-0.114696
C	4.340890	2.680862	-0.021652
C	5.619794	3.240603	-0.214412
C	5.688617	4.618192	-0.515530
H	4.608159	6.444625	-0.845284
H	2.376361	5.412450	-0.518282
H	4.254108	1.621866	0.201166
H	6.656656	5.095397	-0.636669
C	0.826419	3.464163	0.799287
C	1.844332	2.804458	0.091086
C	1.577911	1.526771	-0.422948
C	0.337443	0.898614	-0.239923
C	-0.659594	1.580814	0.476792
C	-0.413153	2.854136	0.987888
H	1.019399	4.445311	1.223534
H	2.337606	1.031896	-1.020822
H	-1.617716	1.100467	0.654639
H	-1.186116	3.367250	1.554017

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IV in the quintet state SCF = -4471.83530827

Mo	10.978882	-0.364483	0.195367
Mo	-10.555316	0.180975	0.409998
I	13.351660	-1.925296	0.118975

I	-13.008907	1.389903	1.099973
P	11.336164	1.078795	-1.836498
P	9.866151	-1.309941	2.244653
P	-9.177014	2.224154	0.102665
P	-11.337899	-2.152614	-0.051724
N	-9.434724	-0.413934	3.210389
N	-9.850704	-0.219232	2.164056
N	9.174404	0.805165	0.231814
N	-8.755183	-0.666825	-0.518176
C	10.257496	2.489828	-1.227257
C	9.053822	2.009699	-0.458178
C	7.896815	2.759076	-0.457978
C	6.743138	2.362054	0.255259
C	6.876774	1.145237	0.961798
C	8.041958	0.408352	0.940338
C	8.119814	-0.892231	1.698459
C	13.008292	1.946287	-2.151158
C	12.880806	3.312903	-2.852618
C	13.647274	2.161067	-0.759382
C	13.931291	1.017612	-2.963403
C	10.533331	0.438555	-3.443451
C	9.034729	0.203640	-3.147073
C	10.649386	1.406800	-4.633045
C	11.176139	-0.919558	-3.797037
C	10.177252	-0.342257	3.858896
C	9.751024	1.121974	3.607794
C	9.398294	-0.877012	5.072550
C	11.693534	-0.360960	4.148088
C	9.769002	-3.193868	2.528995
C	8.505815	-3.650960	3.284529
C	11.036241	-3.664214	3.268881
C	9.766872	-3.842835	1.124740
C	-7.539705	1.326536	0.258975
C	-7.557679	0.010965	-0.468462
C	-6.397391	-0.484772	-1.043525
C	-6.377931	-1.726765	-1.697541

C	-7.604199	-2.405597	-1.746839
C	-8.752791	-1.868949	-1.181090
C	-10.070535	-2.574054	-1.365003
C	-9.203366	2.873055	-1.709872
C	-10.143320	4.085846	-1.845713
C	-7.804023	3.221686	-2.250199
C	-9.789869	1.735287	-2.580048
C	-8.978901	3.663795	1.347563
C	-8.639676	3.036756	2.718978
C	-10.324082	4.404138	1.507244
C	-7.867380	4.655671	0.960239
C	-12.967309	-2.409840	-1.034850
C	-14.156525	-2.407460	-0.054267
C	-13.110725	-1.195252	-1.981513
C	-13.006159	-3.688512	-1.898079
C	-11.112902	-3.508921	1.277413
C	-11.860740	-3.057720	2.549847
C	-11.590316	-4.912726	0.869292
C	-9.598521	-3.585582	1.577805
H	10.921872	3.050796	-0.555906
H	9.959594	3.179009	-2.024832
H	7.877092	3.664781	-1.056540
H	6.054969	0.779884	1.570392
H	7.398299	-0.905648	2.522459
H	7.854037	-1.722909	1.030876
H	12.280553	4.020707	-2.271399
H	12.446521	3.237925	-3.851508
H	13.881507	3.750894	-2.961830
H	13.589948	0.898358	-3.995920
H	14.018094	0.028487	-2.501540
H	14.936233	1.457602	-3.001486
H	13.028018	2.785949	-0.104601
H	14.608660	2.676234	-0.884299
H	13.836684	1.210550	-0.252107
H	8.886395	-0.467495	-2.294733
H	8.500337	1.134544	-2.936168

H	8.570329	-0.258414	-4.027726
H	10.232497	2.393834	-4.402590
H	10.082208	1.002725	-5.481979
H	11.683073	1.535197	-4.964632
H	10.662311	-1.344921	-4.669462
H	12.236097	-0.831907	-4.046098
H	11.090301	-1.632452	-2.969882
H	10.262921	1.553519	2.741576
H	8.673793	1.222151	3.445087
H	10.013558	1.720380	4.489680
H	8.318986	-0.912389	4.885974
H	9.561074	-0.207425	5.927290
H	9.730771	-1.874242	5.372855
H	11.900468	0.264716	5.026555
H	12.070977	-1.364525	4.358085
H	12.266574	0.037152	3.303512
H	7.587296	-3.376301	2.754940
H	8.447884	-3.248091	4.297432
H	8.517063	-4.745660	3.366816
H	11.056539	-3.326371	4.309406
H	11.057239	-4.761582	3.282249
H	11.945753	-3.318985	2.765446
H	9.702900	-4.932956	1.238375
H	10.683274	-3.614729	0.572299
H	8.908699	-3.530124	0.517553
H	-7.449444	1.123268	1.331384
H	-6.671643	1.922814	-0.037803
H	-5.496153	0.117582	-0.991446
H	-7.670802	-3.376779	-2.226984
H	-9.920931	-3.652983	-1.477571
H	-10.509773	-2.220650	-2.306393
H	-11.137496	3.876310	-1.435634
H	-10.266698	4.325300	-2.910145
H	-9.746614	4.979447	-1.357155
H	-7.300885	3.986753	-1.653669
H	-7.894766	3.607565	-3.274357

H	-7.157589	2.338498	-2.292495
H	-9.162012	0.840533	-2.575538
H	-9.867906	2.082399	-3.619375
H	-10.802016	1.456631	-2.256187
H	-9.359885	2.267122	3.007222
H	-8.670157	3.826627	3.480009
H	-7.635847	2.601524	2.750654
H	-10.635549	4.927780	0.602086
H	-10.218282	5.156920	2.299494
H	-11.125982	3.718869	1.795067
H	-6.898670	4.161035	0.824975
H	-7.747447	5.393604	1.764577
H	-8.101330	5.208688	0.046385
H	-14.170635	-3.303867	0.573139
H	-15.094871	-2.392931	-0.624135
H	-14.145924	-1.524961	0.592864
H	-13.188198	-0.254663	-1.430882
H	-14.028909	-1.310879	-2.572343
H	-12.279848	-1.116100	-2.694132
H	-12.189695	-3.724902	-2.627225
H	-13.945078	-3.698964	-2.467195
H	-12.976470	-4.605239	-1.308489
H	-11.522993	-2.078571	2.895039
H	-11.673898	-3.783130	3.352872
H	-12.942100	-3.005801	2.395146
H	-12.675747	-4.963749	0.752265
H	-11.314065	-5.625770	1.657394
H	-11.122620	-5.257431	-0.060042
H	-9.035307	-4.008760	0.738834
H	-9.442995	-4.243302	2.442551
H	-9.169712	-2.612973	1.821805
C	-2.706526	-2.514829	-2.280216
C	-2.788257	-3.277954	-3.457326
C	-4.025363	-3.538896	-4.045547
C	-5.197369	-3.040274	-3.481056
C	-5.147851	-2.270126	-2.305285

C	-3.895084	-2.026812	-1.719417
H	-1.878737	-3.642514	-3.925508
H	-4.073897	-4.117370	-4.964206
H	-6.150587	-3.219144	-3.970000
H	-3.847903	-1.486517	-0.778793
C	1.081694	-1.657305	-0.442470
C	0.857965	-2.898305	-1.036990
C	-0.370588	-3.188045	-1.628971
C	-1.397387	-2.229601	-1.640313
C	-1.154737	-0.984832	-1.040829
C	0.071947	-0.681131	-0.433702
H	2.032405	-1.448200	0.039743
H	1.640287	-3.652529	-1.022611
H	-0.545464	-4.168836	-2.061693
H	-1.919925	-0.215684	-1.088779
C	4.339986	5.279652	0.055236
C	3.109145	4.649732	0.242267
C	3.055239	3.258621	0.438867
C	4.252149	2.532209	0.440963
C	5.505737	3.147718	0.252194
C	5.522740	4.546396	0.060523
H	4.376527	6.355866	-0.093996
H	2.189806	5.226608	0.206401
H	4.206696	1.456851	0.583219
H	6.471198	5.063519	-0.050486
C	0.723621	3.157934	1.375803
C	1.753496	2.567576	0.624343
C	1.517529	1.312811	0.042655
C	0.294479	0.644456	0.196498
C	-0.717054	1.260233	0.951707
C	-0.499440	2.507843	1.534332
H	0.894002	4.117171	1.856003
H	2.284758	0.869245	-0.585187
H	-1.662082	0.745885	1.102698
H	-1.281541	2.968446	2.132235

V in the triplet state SCF = -3548.79273544

Mo	3.264769	0.024225	0.031162
Mo	-3.477366	-0.004690	0.189869
I	3.591270	1.847658	2.205689
I	-3.095856	-1.997088	2.174631
P	3.457124	-2.153390	1.300685
P	3.340232	1.604600	-1.903590
P	-3.554034	-1.493225	-1.779739
P	-2.936502	2.035293	1.535802
N	-6.530264	0.299588	0.394725
N	-5.392641	0.218737	0.319293
N	2.949984	-1.347184	-1.597000
N	-3.265306	1.476857	-1.429344
C	3.853450	-3.192973	-0.214329
C	3.177903	-2.717724	-1.471337
C	2.866859	-3.619214	-2.473985
C	2.364101	-3.183180	-3.708574
C	2.217945	-1.802202	-3.878744
C	2.497476	-0.919794	-2.846899
C	2.287019	0.557478	-3.053265
C	4.994127	-2.442501	2.395443
C	5.480882	-3.905314	2.417343
C	6.117095	-1.552669	1.813547
C	4.697991	-1.967724	3.830818
C	1.877915	-2.906804	2.050540
C	0.834201	-2.899638	0.914214
C	2.044397	-4.344889	2.568212
C	1.372065	-1.993707	3.186815
C	5.049867	1.755336	-2.738637
C	5.486645	0.334208	-3.159583
C	5.064719	2.656875	-3.984901
C	6.054117	2.281154	-1.690609
C	2.397457	3.267321	-1.904965
C	1.894043	3.716923	-3.290662
C	3.279105	4.358787	-1.268185

C	1.172973	3.057771	-0.988057
C	-4.217716	-0.198385	-2.959221
C	-3.582064	1.142425	-2.728209
C	-3.357688	2.004505	-3.796492
C	-2.826977	3.274779	-3.576775
C	-2.522068	3.626110	-2.264430
C	-2.730895	2.724988	-1.222222
C	-2.244101	3.085065	0.154968
C	-1.773827	-1.862512	-2.389628
C	-1.299266	-3.248071	-1.910506
C	-1.592375	-1.738531	-3.912851
C	-0.879031	-0.807335	-1.695814
C	-4.719316	-2.973796	-2.088382
C	-6.170786	-2.471632	-1.911831
C	-4.473750	-4.051610	-1.011389
C	-4.569040	-3.581449	-3.494962
C	-1.415051	1.985471	2.701041
C	-1.830198	1.426650	4.075507
C	-0.420666	0.997768	2.049100
C	-0.685211	3.333367	2.890538
C	-4.342515	3.098110	2.266089
C	-5.177843	2.207499	3.210274
C	-3.876338	4.353241	3.023294
C	-5.224723	3.548463	1.079261
H	4.938057	-3.068677	-0.335850
H	3.674095	-4.260681	-0.051816
H	3.043440	-4.675959	-2.293684
H	2.125805	-3.881805	-4.502867
H	1.871148	-1.396893	-4.825584
H	2.407734	0.820976	-4.110318
H	1.259239	0.828522	-2.780238
H	5.776270	-4.260179	1.424323
H	4.731564	-4.592978	2.815213
H	6.367035	-3.975393	3.061845
H	4.012816	-2.644958	4.348733
H	4.275786	-0.957228	3.845680

H	5.634795	-1.948765	4.402689
H	6.341828	-1.790682	0.766402
H	7.038064	-1.716480	2.388774
H	5.863579	-0.489788	1.878741
H	0.699906	-1.897533	0.496242
H	1.107848	-3.569962	0.093460
H	-0.136313	-3.218180	1.311998
H	2.443518	-5.021513	1.803702
H	1.061296	-4.730874	2.867291
H	2.694359	-4.393471	3.446648
H	0.342115	-2.272217	3.442158
H	1.978802	-2.080555	4.091087
H	1.370151	-0.943644	2.887294
H	5.478071	-0.361386	-2.314767
H	4.847679	-0.083192	-3.943832
H	6.510877	0.381367	-3.551476
H	4.334916	2.332538	-4.735301
H	6.057547	2.609187	-4.451263
H	4.870012	3.704863	-3.742752
H	7.059905	2.299745	-2.131334
H	5.819400	3.293801	-1.353870
H	6.081686	1.637576	-0.804561
H	1.203010	2.990675	-3.731840
H	2.703684	3.894891	-4.000580
H	1.341193	4.659343	-3.178694
H	4.116768	4.644262	-1.911205
H	2.672757	5.259539	-1.105208
H	3.670703	4.040095	-0.295920
H	0.580346	3.982319	-0.973650
H	1.473926	2.829565	0.038273
H	0.511853	2.258785	-1.344031
H	-5.278177	-0.121886	-2.695461
H	-4.158766	-0.481688	-4.014588
H	-3.621670	1.676320	-4.797105
H	-2.657742	3.963931	-4.398021
H	-2.096107	4.597841	-2.033444

H	-2.364448	4.157878	0.339755
H	-1.167527	2.896473	0.175599
H	-1.432613	-3.365155	-0.830067
H	-0.229536	-3.353530	-2.131316
H	-1.820710	-4.064881	-2.416792
H	-2.219633	-2.441698	-4.468239
H	-0.546836	-1.951216	-4.168060
H	-1.817439	-0.725235	-4.264001
H	-1.061195	0.204233	-2.069744
H	0.172074	-1.053551	-1.875109
H	-1.018806	-0.811062	-0.604912
H	-6.315958	-1.946837	-0.963968
H	-6.842750	-3.339201	-1.919176
H	-6.491185	-1.813621	-2.726140
H	-3.477782	-4.493486	-1.070193
H	-5.202427	-4.861211	-1.150302
H	-4.600855	-3.645469	-0.004552
H	-4.720039	-2.836800	-4.284904
H	-5.327410	-4.363546	-3.632959
H	-3.591094	-4.047022	-3.645088
H	-2.433694	2.143673	4.641349
H	-0.927927	1.219792	4.665539
H	-2.391303	0.491695	3.981625
H	-0.796864	-0.027384	2.067288
H	0.525508	1.030183	2.598837
H	-0.177283	1.258500	1.011873
H	-0.336426	3.761332	1.945175
H	0.210051	3.160133	3.500457
H	-1.293328	4.081274	3.401397
H	-5.557275	1.318610	2.702067
H	-6.038979	2.781097	3.578457
H	-4.602070	1.879144	4.080502
H	-3.352220	4.105913	3.950149
H	-4.755198	4.952409	3.296692
H	-3.222871	4.990134	2.416206
H	-4.709631	4.270471	0.435354

H	-6.121207	4.044525	1.473272
H	-5.555930	2.712193	0.461925

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V in the quintet state SCF = -3548.79280291

Mo	3.248096	0.043097	0.041604
Mo	-3.465117	-0.029722	0.172073
I	3.522417	1.921997	2.173664
I	-3.094723	-1.992853	2.186187
P	3.466497	-2.098428	1.368548
P	3.320091	1.579486	-1.928623
P	-3.479897	-1.540474	-1.782512
P	-2.991275	2.038630	1.504719
N	-6.526238	0.228118	0.301659
N	-5.385985	0.164447	0.253961
N	2.984591	-1.372331	-1.558188
N	-3.237723	1.437124	-1.459538
C	3.896886	-3.169208	-0.114936
C	3.233809	-2.735554	-1.393897
C	2.956109	-3.667193	-2.378620
C	2.470230	-3.271333	-3.633295
C	2.305365	-1.897710	-3.841396
C	2.549363	-0.984703	-2.827454
C	2.318104	0.483052	-3.077857
C	4.997533	-2.326832	2.486421
C	5.508404	-3.779505	2.559944
C	6.112315	-1.438075	1.887423
C	4.677785	-1.810780	3.902326
C	1.895391	-2.861431	2.125804
C	0.865735	-2.914246	0.978285
C	2.085312	-4.278232	2.692027
C	1.357592	-1.921954	3.225033
C	5.039278	1.757060	-2.737633
C	5.520554	0.337279	-3.111785
C	5.049124	2.625011	-4.007405
C	6.010635	2.337886	-1.687945

C	2.334455	3.216302	-1.978691
C	1.836382	3.619566	-3.380531
C	3.177811	4.346944	-1.358549
C	1.105653	2.994448	-1.070366
C	-4.134293	-0.267271	-2.990524
C	-3.520549	1.083977	-2.761202
C	-3.283124	1.936804	-3.834151
C	-2.775961	3.217187	-3.617126
C	-2.506392	3.587565	-2.302328
C	-2.724606	2.694579	-1.255086
C	-2.271164	3.074016	0.127731
C	-1.682934	-1.893475	-2.350419
C	-1.203902	-3.271288	-1.853753
C	-1.469927	-1.775099	-3.869902
C	-0.816092	-0.824750	-1.642277
C	-4.618594	-3.039408	-2.100646
C	-6.080417	-2.555648	-1.962708
C	-4.383062	-4.102086	-1.006389
C	-4.429231	-3.659622	-3.497149
C	-1.504854	2.031097	2.715619
C	-1.955648	1.488995	4.085403
C	-0.475856	1.048263	2.111901
C	-0.802519	3.393710	2.903270
C	-4.435560	3.095022	2.169436
C	-5.290570	2.211029	3.102120
C	-4.011203	4.369550	2.918820
C	-5.281609	3.511072	0.944584
H	4.981356	-3.033781	-0.224735
H	3.729301	-4.235055	0.071204
H	3.146663	-4.715933	-2.168097
H	2.258453	-3.993767	-4.413670
H	1.971905	-1.522129	-4.805122
H	2.465887	0.722082	-4.137334
H	1.277798	0.742494	-2.844407
H	5.815483	-4.162102	1.580804
H	4.768744	-4.466365	2.976574

H	6.391865	-3.813285	3.211079
H	4.000573	-2.483719	4.436185
H	4.235998	-0.808802	3.879144
H	5.607994	-1.754143	4.482504
H	6.353275	-1.707457	0.851562
H	7.028886	-1.567529	2.478179
H	5.841446	-0.377868	1.914097
H	0.716704	-1.930023	0.524867
H	1.163490	-3.606520	0.184584
H	-0.103234	-3.239002	1.375147
H	2.509011	-4.970332	1.954991
H	1.106452	-4.675244	2.990565
H	2.723936	-4.284649	3.579804
H	0.334266	-2.219454	3.485746
H	1.961612	-1.957218	4.134670
H	1.327678	-0.884478	2.885831
H	5.516795	-0.334398	-2.247663
H	4.905172	-0.118885	-3.893344
H	6.549286	0.401125	-3.489292
H	4.341164	2.259889	-4.760015
H	6.050361	2.593832	-4.456934
H	4.820406	3.672941	-3.796473
H	7.023625	2.369179	-2.111115
H	5.744771	3.353356	-1.384751
H	6.037221	1.720478	-0.783520
H	1.168490	2.866194	-3.811596
H	2.650142	3.799609	-4.085445
H	1.259518	4.550546	-3.298394
H	4.014281	4.641550	-1.999170
H	2.544029	5.233386	-1.223527
H	3.566832	4.062925	-0.374513
H	0.478107	3.895113	-1.099930
H	1.400591	2.817026	-0.032010
H	0.480506	2.157186	-1.402833
H	-5.201118	-0.200950	-2.750550
H	-4.049045	-0.561681	-4.040998

H	-3.519378	1.593549	-4.836642
H	-2.597743	3.899484	-4.442190
H	-2.099894	4.567907	-2.072763
H	-2.398827	4.148645	0.295961
H	-1.194828	2.887796	0.175983
H	-1.359306	-3.383597	-0.775899
H	-0.128792	-3.366841	-2.051236
H	-1.705149	-4.096662	-2.366407
H	-2.079931	-2.485594	-4.435168
H	-0.417931	-1.981279	-4.101479
H	-1.694943	-0.765148	-4.230614
H	-0.994334	0.180758	-2.033839
H	0.241824	-1.066478	-1.784022
H	-0.988831	-0.815550	-0.556167
H	-6.255082	-2.024133	-1.023763
H	-6.740000	-3.432597	-1.977473
H	-6.390556	-1.909872	-2.790657
H	-3.380890	-4.532536	-1.039000
H	-5.098957	-4.921964	-1.151348
H	-4.536455	-3.686145	-0.007123
H	-4.575042	-2.925866	-4.298234
H	-5.172491	-4.454797	-3.642329
H	-3.441412	-4.111282	-3.622168
H	-2.591947	2.203759	4.617240
H	-1.070355	1.310163	4.709316
H	-2.495110	0.541533	3.989355
H	-0.836716	0.017878	2.138552
H	0.454321	1.106781	2.686663
H	-0.205441	1.292540	1.077372
H	-0.420947	3.804143	1.962714
H	0.068800	3.247729	3.553774
H	-1.441559	4.144011	3.370632
H	-5.645146	1.310038	2.597588
H	-6.168674	2.781389	3.433510
H	-4.739185	1.903632	3.995602
H	-3.508071	4.145187	3.863203

H	-4.907042	4.957955	3.158466
H	-3.352000	5.007718	2.319262
H	-4.755558	4.232152	0.308613
H	-6.200851	3.996214	1.297454
H	-5.573403	2.659055	0.328670

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TS_{II/VI} in the closed-shell singlet state SCF = -4471.85870329

Mo	1.836746	2.401373	0.314531
Mo	1.586954	-2.484463	-0.395436
I	4.087718	3.097040	2.041237
I	3.678818	-3.618700	-2.041317
P	2.913352	2.893036	-1.848110
P	0.191190	3.245351	2.031745
P	2.770863	-3.034723	1.701775
P	-0.355075	-2.954184	-1.995749
N	1.769481	0.667707	0.377410
N	1.683434	-0.767830	-0.307315
N	0.069519	2.890129	-0.909548
N	-0.038542	-2.955022	0.988924
C	1.444736	3.535672	-2.836681
C	0.123357	3.102359	-2.266369
C	-0.993618	2.979112	-3.077884
C	-2.269965	2.710851	-2.539370
C	-2.328137	2.717446	-1.137759
C	-1.181545	2.771267	-0.361980
C	-1.314602	2.602466	1.131110
C	4.124935	4.372063	-2.044716
C	4.209194	4.953527	-3.472138
C	3.617963	5.492474	-1.107821
C	5.529202	3.937311	-1.582751
C	3.512960	1.377560	-2.849957
C	2.250846	0.548341	-3.173962
C	4.220861	1.697342	-4.177712
C	4.455062	0.552578	-1.947644
C	-0.088877	5.136722	2.152594

C	-0.363885	5.672161	0.728960
C	-1.274884	5.523284	3.053489
C	1.202916	5.810635	2.660534
C	0.024950	2.413587	3.743729
C	0.908969	3.137182	4.777418
C	0.574083	0.983903	3.568673
C	-1.427890	2.318741	4.254561
C	1.468384	-2.242868	2.796604
C	0.085919	-2.569040	2.299965
C	-1.029799	-2.443879	3.125089
C	-2.311511	-2.737740	2.639938
C	-2.393148	-3.295359	1.353615
C	-1.257113	-3.426213	0.573256
C	-1.278940	-4.058073	-0.781631
C	2.785908	-4.903369	2.176376
C	4.123128	-5.541103	1.747838
C	2.532292	-5.134722	3.678441
C	1.669679	-5.628363	1.388866
C	4.389018	-2.192469	2.276424
C	4.141128	-0.670957	2.326582
C	5.481141	-2.445529	1.214985
C	4.874622	-2.636795	3.669336
C	-0.282974	-4.062659	-3.561729
C	0.664643	-3.397348	-4.583421
C	0.331796	-5.417728	-3.139916
C	-1.643207	-4.348680	-4.224512
C	-1.604909	-1.520414	-2.254698
C	-1.276963	-0.783457	-3.566597
C	-3.080942	-1.977218	-2.271474
C	-1.462196	-0.516325	-1.092169
H	1.478972	4.628588	-2.747993
H	1.514945	3.307574	-3.904286
H	-0.850719	3.082305	-4.147192
H	-3.264590	2.567917	-0.615665
H	-2.268060	3.017951	1.478009
H	-1.328674	1.528931	1.361474

H	3.238121	5.295606	-3.846310
H	4.623949	4.251501	-4.195781
H	4.870626	5.830030	-3.453788
H	5.980485	3.219462	-2.274124
H	5.508272	3.496071	-0.582531
H	6.186298	4.816676	-1.546920
H	2.609824	5.836977	-1.372471
H	4.287448	6.359040	-1.192342
H	3.612646	5.176410	-0.062360
H	1.625948	0.394603	-2.295237
H	1.650982	1.016712	-3.963725
H	2.554644	-0.445715	-3.524569
H	3.607463	2.322475	-4.837355
H	4.411719	0.753363	-4.704903
H	5.186343	2.188620	-4.030733
H	4.734129	-0.373530	-2.464112
H	5.371321	1.099974	-1.704476
H	3.965916	0.273314	-1.014210
H	0.445820	5.421068	0.036713
H	-1.301741	5.295529	0.308827
H	-0.438017	6.766283	0.775905
H	-2.207576	5.039002	2.742467
H	-1.433355	6.608175	2.993851
H	-1.092629	5.279282	4.103027
H	1.063729	6.899981	2.644894
H	1.459211	5.523780	3.681884
H	2.061502	5.563959	2.030378
H	0.514417	4.121184	5.046849
H	1.936150	3.252441	4.415778
H	0.940503	2.537187	5.696612
H	1.630359	1.000793	3.289712
H	0.469553	0.442546	4.519098
H	0.032627	0.420286	2.802263
H	-1.424018	1.824481	5.235106
H	-2.058380	1.714084	3.594190
H	-1.903241	3.293326	4.382296

H	1.650953	-1.176619	2.647638
H	1.555736	-2.443478	3.870265
H	-0.902594	-2.060899	4.132809
H	-3.349862	-3.629731	0.965826
H	-2.293945	-4.308944	-1.098832
H	-0.704291	-4.990397	-0.733034
H	4.323334	-5.372988	0.684430
H	4.067705	-6.625562	1.911781
H	4.972006	-5.168850	2.324874
H	3.270487	-4.644067	4.315551
H	2.577519	-6.211631	3.889516
H	1.536713	-4.787191	3.976335
H	0.670668	-5.283218	1.666982
H	1.723977	-6.702631	1.610946
H	1.795632	-5.506634	0.307041
H	3.648692	-0.285818	1.432966
H	5.104322	-0.156694	2.413728
H	3.548483	-0.369964	3.196409
H	5.707413	-3.502676	1.064884
H	6.404038	-1.947281	1.539776
H	5.192762	-2.031127	0.245899
H	4.106353	-2.485273	4.436438
H	5.739001	-2.021196	3.950062
H	5.195611	-3.681034	3.701851
H	0.266230	-2.456888	-4.970382
H	0.798795	-4.074506	-5.437548
H	1.649236	-3.207106	-4.149888
H	1.257933	-5.296999	-2.571937
H	0.579533	-5.986563	-4.045069
H	-0.371138	-6.027057	-2.560564
H	-2.358696	-4.797706	-3.526168
H	-1.493275	-5.065731	-5.042735
H	-2.096820	-3.454082	-4.658926
H	-0.224392	-0.490705	-3.612228
H	-1.879149	0.127156	-3.621583
H	-1.513709	-1.382042	-4.450104

H	-3.292540	-2.758840	-3.001808
H	-3.709423	-1.112800	-2.523643
H	-3.401213	-2.330793	-1.285494
H	-1.566956	-0.988186	-0.112423
H	-2.262028	0.222816	-1.192820
H	-0.507289	0.008803	-1.107827
C	-5.798627	-1.513987	3.483063
C	-5.928538	-2.007664	4.795224
C	-4.879328	-2.681941	5.417887
C	-3.680710	-2.906766	4.742936
C	-3.541045	-2.474625	3.416409
C	-4.596132	-1.776088	2.809001
H	-6.862191	-1.878004	5.332715
H	-5.005319	-3.048641	6.432945
H	-2.869251	-3.447740	5.221771
H	-4.443923	-1.394193	1.803972
C	-8.927407	0.837879	1.680623
C	-8.824724	0.739969	3.065971
C	-7.806380	-0.012471	3.645822
C	-6.882677	-0.713387	2.849508
C	-7.006195	-0.607090	1.452608
C	-8.005107	0.175406	0.854257
H	-9.695575	1.462088	1.233529
H	-9.524822	1.277442	3.699853
H	-7.713187	-0.029281	4.726657
H	-6.331411	-1.162464	0.807945
C	-4.377570	1.521101	-5.462719
C	-5.553076	1.132850	-4.820875
C	-5.708554	1.356870	-3.441423
C	-4.650528	1.957336	-2.748773
C	-3.429695	2.298877	-3.359479
C	-3.325735	2.091779	-4.749453
H	-4.266658	1.349305	-6.529896
H	-6.335806	0.634930	-5.384676
H	-4.795009	2.163635	-1.696652
H	-2.410235	2.336999	-5.276619

C	-8.198588	0.978035	-3.359069
C	-6.949422	0.973954	-2.716212
C	-6.910314	0.642432	-1.351161
C	-8.073439	0.371010	-0.618193
C	-9.305571	0.373957	-1.292192
C	-9.360137	0.665113	-2.654176
H	-8.267179	1.260861	-4.405109
H	-5.956944	0.621903	-0.831964
H	-10.215920	0.140209	-0.747581
H	-10.317901	0.667614	-3.167502

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TS_{II/VI} in the triplet state SCF = -4471.84420466

Mo	1.679174	-2.455946	-0.168638
Mo	1.736360	2.402109	0.244757
I	3.794212	-3.267056	-1.887610
I	3.872583	3.589187	1.796847
P	2.849499	-2.721381	2.056681
P	-0.059238	-3.407863	-1.852377
P	2.889838	2.770994	-1.909336
P	-0.186062	3.062300	1.822511
N	1.495503	-0.728218	-0.486242
N	1.791776	0.679081	0.173578
N	-0.031906	-2.866650	1.075783
N	0.093283	2.740217	-1.149801
C	1.376842	-3.292048	3.061223
C	0.049884	-2.888102	2.474024
C	-1.030688	-2.653039	3.286636
C	-2.341969	-2.428667	2.768966
C	-2.430108	-2.619825	1.357404
C	-1.324021	-2.767881	0.565887
C	-1.501546	-2.702749	-0.933937
C	4.041509	-4.213992	2.263302
C	4.162455	-4.698502	3.725365
C	3.479665	-5.387158	1.427335

C	5.440352	-3.847758	1.731451
C	3.528030	-1.172276	2.931435
C	2.295332	-0.293056	3.230476
C	4.275478	-1.413551	4.253162
C	4.454972	-0.448525	1.932566
C	-0.313737	-5.303414	-1.819203
C	-0.516973	-5.732677	-0.347873
C	-1.546141	-5.749205	-2.627790
C	0.947582	-6.018722	-2.345778
C	-0.264670	-2.698789	-3.615398
C	0.538524	-3.525435	-4.637490
C	0.337375	-1.280956	-3.570079
C	-1.739233	-2.598673	-4.057494
C	1.575516	1.861024	-2.896467
C	0.202477	2.257273	-2.428630
C	-0.914732	2.119194	-3.249413
C	-2.184711	2.493844	-2.792613
C	-2.245143	3.145672	-1.550190
C	-1.105395	3.290367	-0.777603
C	-1.096560	4.051709	0.508459
C	2.879574	4.585049	-2.550169
C	4.227620	5.262955	-2.230052
C	2.569726	4.678856	-4.056585
C	1.788013	5.375460	-1.790251
C	4.500297	1.880965	-2.435405
C	4.268562	0.363201	-2.290721
C	5.635170	2.264658	-1.462461
C	4.915573	2.163631	-3.891183
C	-0.062401	4.335475	3.254324
C	0.863697	3.758215	4.346905
C	0.592787	5.614253	2.683819
C	-1.413388	4.731202	3.878038
C	-1.468191	1.696430	2.247637
C	-1.155829	1.105423	3.635001
C	-2.933320	2.185808	2.214131
C	-1.349438	0.570251	1.201536

H	1.425456	-4.387806	3.057858
H	1.461157	-2.978830	4.106016
H	-0.856915	-2.652500	4.357859
H	-3.383883	-2.542747	0.848755
H	-2.460265	-3.142783	-1.227506
H	-1.523724	-1.646391	-1.235047
H	3.197515	-4.987487	4.154573
H	4.621074	-3.960730	4.383459
H	4.801335	-5.591198	3.742499
H	5.931539	-3.097480	2.357767
H	5.402051	-3.475668	0.704285
H	6.073041	-4.745173	1.737032
H	2.468200	-5.677389	1.736133
H	4.125460	-6.263588	1.570234
H	3.463489	-5.160829	0.359589
H	1.641837	-0.193093	2.363998
H	1.712358	-0.690126	4.068883
H	2.630640	0.717435	3.492438
H	3.672827	-1.976297	4.975165
H	4.503132	-0.438913	4.704032
H	5.225901	-1.934553	4.109034
H	4.805015	0.490463	2.376023
H	5.330447	-1.050715	1.671193
H	3.922631	-0.187886	1.017120
H	0.324299	-5.437497	0.285799
H	-1.427319	-5.315733	0.092141
H	-0.597662	-6.826792	-0.315185
H	-2.462785	-5.249133	-2.295996
H	-1.694503	-6.827844	-2.487041
H	-1.425372	-5.575874	-3.700175
H	0.806957	-7.102860	-2.242848
H	1.147444	-5.810802	-3.398361
H	1.839250	-5.735474	-1.780584
H	0.097524	-4.509559	-4.817949
H	1.578679	-3.656926	-4.322824
H	0.543788	-2.990294	-5.596063

H	1.409279	-1.314430	-3.358919
H	0.188478	-0.799486	-4.546490
H	-0.131216	-0.650721	-2.809314
H	-1.774869	-2.191680	-5.076631
H	-2.314628	-1.919407	-3.420557
H	-2.247101	-3.565716	-4.072582
H	1.748416	0.817034	-2.624733
H	1.659120	1.942025	-3.985727
H	-0.799033	1.663979	-4.227793
H	-3.186950	3.548564	-1.192659
H	-2.101266	4.359263	0.807977
H	-0.500458	4.959055	0.356934
H	4.471243	5.185535	-1.164802
H	4.156255	6.329225	-2.482110
H	5.055923	4.848042	-2.808583
H	3.291737	4.142214	-4.675511
H	2.591684	5.733090	-4.363250
H	1.569181	4.294281	-4.284171
H	0.781039	5.009963	-2.005127
H	1.833054	6.426816	-2.104347
H	1.948787	5.347815	-0.706332
H	3.837797	0.092151	-1.326303
H	5.232593	-0.150897	-2.377066
H	3.623746	-0.047756	-3.073072
H	5.866483	3.330877	-1.461271
H	6.544896	1.726168	-1.759564
H	5.389415	1.980774	-0.436469
H	4.115511	1.918207	-4.599104
H	5.776957	1.530840	-4.141439
H	5.216626	3.201570	-4.054942
H	0.440114	2.873466	4.827721
H	1.009027	4.518170	5.126481
H	1.846605	3.502268	3.944451
H	1.502937	5.400508	2.116763
H	0.877935	6.266436	3.518994
H	-0.098451	6.185115	2.053496

H	-2.119753	5.114031	3.132716
H	-1.244522	5.533690	4.608437
H	-1.888611	3.903252	4.410385
H	-0.107341	0.809755	3.723157
H	-1.768066	0.212400	3.784347
H	-1.392199	1.801115	4.444610
H	-3.124365	3.048119	2.853998
H	-3.577453	1.367965	2.561908
H	-3.250297	2.433254	1.195195
H	-1.460474	0.932004	0.176332
H	-2.152127	-0.145439	1.391414
H	-0.403576	0.033910	1.262766
C	-5.721783	1.366462	-3.553317
C	-5.824975	1.751188	-4.903629
C	-4.744268	2.322097	-5.574286
C	-3.538505	2.550175	-4.912921
C	-3.422146	2.224217	-3.554173
C	-4.508812	1.626798	-2.897391
H	-6.762570	1.618433	-5.433549
H	-4.850806	2.607141	-6.617455
H	-2.703188	3.013950	-5.430348
H	-4.376661	1.321983	-1.863726
C	-8.949249	-0.662089	-1.548160
C	-8.848675	-0.696255	-2.937010
C	-7.800101	-0.047610	-3.585035
C	-6.843232	0.680126	-2.855128
C	-6.968117	0.711861	-1.455171
C	-7.996167	0.032253	-0.785074
H	-9.741161	-1.209438	-1.045445
H	-9.574916	-1.258277	-3.518170
H	-7.710033	-0.135112	-4.662949
H	-6.267867	1.294815	-0.864723
C	-4.339705	-0.887058	5.590801
C	-5.508917	-0.495270	4.932532
C	-5.683526	-0.829765	3.575306
C	-4.664270	-1.528407	2.923234

C	-3.440904	-1.882245	3.545222
C	-3.325643	-1.565503	4.924484
H	-4.209064	-0.637160	6.641000
H	-6.261163	0.084024	5.458502
H	-4.831673	-1.812317	1.892651
H	-2.423445	-1.822600	5.470160
C	-8.162598	-0.372889	3.483488
C	-6.920812	-0.468017	2.832255
C	-6.893094	-0.261831	1.442417
C	-8.057393	-0.024785	0.699333
C	-9.281306	0.071161	1.381248
C	-9.324154	-0.090799	2.765130
H	-8.224478	-0.555941	4.551855
H	-5.945834	-0.320400	0.915500
H	-10.191939	0.281036	0.827097
H	-10.274449	-0.016415	3.287398

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VI in the closed-shell singlet state SCF = -4471.93825086

Mo	-0.494394	3.692818	0.213737
Mo	-2.948347	-2.676923	0.095528
I	-1.530493	6.095230	-1.017168
I	-5.205877	-4.466396	0.211854
P	-1.374174	4.018509	2.540962
P	1.385358	3.440287	-1.385898
P	-3.803382	-1.436669	-1.894290
P	-1.242333	-4.078302	1.312557
N	-1.408688	2.463631	-0.422801
N	-3.154927	-1.393126	1.123404
N	0.937476	2.469441	1.396556
N	-1.094744	-2.307822	-1.107071
C	0.137617	3.440874	3.511006
C	0.968163	2.435653	2.761134
C	1.764345	1.532540	3.457906
C	2.574191	0.617019	2.773063
C	2.549897	0.685420	1.372951

C	1.755921	1.612309	0.710285
C	1.811728	1.701962	-0.794248
C	-1.655236	5.733962	3.344894
C	-1.568872	5.755650	4.885108
C	-0.548448	6.661889	2.791681
C	-3.021903	6.274584	2.882083
C	-2.733700	2.757950	3.001928
C	-2.148677	1.344872	2.790495
C	-3.223200	2.870576	4.455996
C	-3.921365	2.953284	2.037613
C	2.958706	4.481787	-1.061622
C	3.364350	4.328732	0.422473
C	4.158030	4.064367	-1.930332
C	2.622048	5.971698	-1.292156
C	1.101937	3.193329	-3.263809
C	1.194834	4.542200	-4.003770
C	-0.346397	2.680086	-3.414709
C	2.066278	2.170744	-3.898315
C	-2.249512	-0.392188	-2.109908
C	-1.040867	-1.267099	-1.998200
C	0.080410	-1.055069	-2.798899
C	1.210830	-1.871900	-2.681876
C	1.133101	-2.940068	-1.775235
C	-0.027928	-3.160932	-1.045922
C	-0.194993	-4.400841	-0.217876
C	-3.928432	-2.432538	-3.530742
C	-5.378710	-2.914922	-3.734186
C	-3.446102	-1.644448	-4.763634
C	-3.040834	-3.692815	-3.389224
C	-5.182598	-0.123439	-1.757457
C	-4.749106	0.903151	-0.688292
C	-6.465255	-0.820745	-1.256605
C	-5.446775	0.632258	-3.072262
C	-1.512186	-5.857190	1.988637
C	-2.636060	-5.779127	3.045057
C	-2.010888	-6.731897	0.815398

C	-0.270802	-6.540088	2.590423
C	-0.036607	-3.111142	2.461103
C	-0.529751	-3.194313	3.919382
C	1.420535	-3.610742	2.358416
C	-0.041944	-1.621698	2.061002
H	0.746741	4.339241	3.668092
H	-0.119376	3.062666	4.505628
H	1.754627	1.552676	4.542640
H	3.129337	-0.013202	0.780256
H	2.766306	1.310300	-1.163337
H	1.016399	1.082686	-1.226165
H	-0.603421	5.392238	5.254966
H	-2.357522	5.176039	5.365980
H	-1.672850	6.793938	5.226909
H	-3.852692	5.722221	3.332254
H	-3.120411	6.237609	1.792138
H	-3.119519	7.323388	3.191696
H	0.460188	6.321174	3.059440
H	-0.672473	7.661421	3.228375
H	-0.606055	6.765108	1.705723
H	-1.764745	1.203990	1.778254
H	-1.351653	1.117287	3.508106
H	-2.941713	0.602082	2.928406
H	-2.403663	2.805432	5.181086
H	-3.906063	2.036013	4.659400
H	-3.777118	3.795791	4.637891
H	-4.677018	2.185157	2.244579
H	-4.395406	3.932072	2.154707
H	-3.607189	2.846614	0.997940
H	2.560065	4.623906	1.103784
H	3.669765	3.309574	0.676470
H	4.219789	4.987806	0.618112
H	4.404542	3.003076	-1.810087
H	5.041677	4.643675	-1.631562
H	3.984686	4.259011	-2.991040
H	3.484447	6.582062	-0.992586

H	2.404134	6.200388	-2.336111
H	1.755085	6.287851	-0.702979
H	2.219074	4.922106	-4.060083
H	0.557145	5.300872	-3.538138
H	0.845271	4.399849	-5.034780
H	-1.073338	3.428044	-3.088173
H	-0.528148	2.446521	-4.473057
H	-0.533212	1.782131	-2.823854
H	1.817166	2.058647	-4.961901
H	1.982670	1.179208	-3.445608
H	3.113785	2.475164	-3.842343
H	-2.253713	0.320778	-1.277270
H	-2.225548	0.195800	-3.031354
H	0.072791	-0.234800	-3.506759
H	1.956384	-3.641450	-1.688123
H	0.768483	-4.873788	-0.008776
H	-0.780191	-5.116273	-0.808287
H	-5.748178	-3.452477	-2.854693
H	-5.407530	-3.605971	-4.587052
H	-6.063681	-2.093238	-3.957087
H	-4.000743	-0.716625	-4.919782
H	-3.578238	-2.264688	-5.660197
H	-2.380392	-1.399298	-4.693073
H	-1.981232	-3.446405	-3.278008
H	-3.142366	-4.300141	-4.298635
H	-3.354024	-4.315085	-2.543183
H	-4.447209	0.420868	0.244763
H	-5.605034	1.555859	-0.473345
H	-3.929781	1.545632	-1.024695
H	-6.868763	-1.540628	-1.971750
H	-7.236169	-0.058417	-1.082593
H	-6.285476	-1.351560	-0.317402
H	-4.541078	1.119336	-3.451276
H	-6.185188	1.422501	-2.884776
H	-5.851049	-0.011918	-3.857692
H	-2.344850	-5.197798	3.923806

H	-2.876323	-6.794334	3.387924
H	-3.545818	-5.340959	2.625853
H	-2.820977	-6.257321	0.254628
H	-2.407368	-7.670877	1.222039
H	-1.200489	-6.998226	0.126822
H	0.555167	-6.603475	1.872662
H	-0.534647	-7.568114	2.872801
H	0.092228	-6.040299	3.492080
H	-1.569822	-2.862212	4.007311
H	0.088251	-2.531346	4.539409
H	-0.449406	-4.200063	4.339271
H	1.534610	-4.675884	2.564268
H	2.035349	-3.067144	3.084238
H	1.841848	-3.404258	1.368370
H	0.330939	-1.461425	1.045194
H	0.625690	-1.085571	2.742432
H	-1.034649	-1.177740	2.126643
C	4.872882	-1.650333	-3.679166
C	4.738452	-1.438508	-5.063520
C	3.480845	-1.308362	-5.652110
C	2.321982	-1.417556	-4.886020
C	2.421235	-1.669895	-3.508993
C	3.691974	-1.760158	-2.925301
H	5.620084	-1.389488	-5.694029
H	3.405237	-1.142056	-6.723054
H	1.344241	-1.345143	-5.353534
H	3.744944	-1.889547	-1.849357
C	8.696914	-1.761484	-1.682061
C	8.594934	-1.251197	-2.976240
C	7.364516	-1.205401	-3.630183
C	6.207851	-1.726701	-3.022148
C	6.345118	-2.281540	-1.741181
C	7.557059	-2.262073	-1.035638
H	9.645407	-1.722930	-1.154111
H	9.475655	-0.843099	-3.464587
H	7.304922	-0.732737	-4.605024

H	5.487513	-2.744319	-1.265969
C	3.709807	-2.072577	5.194822
C	4.848006	-2.554992	4.544976
C	5.292683	-1.957935	3.353414
C	4.562129	-0.870001	2.856509
C	3.381939	-0.415981	3.456259
C	2.968642	-1.020003	4.655721
H	3.373320	-2.549917	6.110888
H	5.373852	-3.414921	4.949154
H	4.930271	-0.345626	1.982765
H	2.048298	-0.702851	5.137098
C	7.569283	-3.081973	3.184646
C	6.465507	-2.452950	2.586860
C	6.493824	-2.262972	1.198979
C	7.583174	-2.634066	0.402463
C	8.672316	-3.262979	1.025338
C	8.652861	-3.489140	2.403209
H	7.598227	-3.224554	4.261061
H	5.650444	-1.782840	0.717698
H	9.524807	-3.583795	0.433206
H	9.500272	-3.976506	2.877652

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VI in the triplet state SCF = -4471.91874080

Mo	-1.951634	-3.043362	-0.135218
Mo	-1.629215	3.506099	-0.208382
I	-4.187277	-4.321239	1.184085
I	-3.002358	5.921278	-0.541999
P	-2.802217	-3.148214	-2.498620
P	-0.274783	-3.705328	1.565549
P	-2.928400	2.847785	1.899462
P	0.581095	3.903863	-1.466370
N	-2.058783	-1.452874	0.323192
N	-2.297465	2.374498	-1.220365
N	-0.050941	-2.897365	-1.283418
N	-0.093606	2.727230	1.162602

C	-1.171169	-3.521122	-3.376714
C	0.020421	-2.971389	-2.643808
C	1.152653	-2.570006	-3.341431
C	2.279020	-2.080741	-2.661882
C	2.220724	-2.105340	-1.261368
C	1.070269	-2.516572	-0.596851
C	1.044761	-2.530263	0.912727
C	-3.883551	-4.582174	-3.162390
C	-3.762776	-4.844112	-4.677666
C	-3.419845	-5.856792	-2.418531
C	-5.353100	-4.306042	-2.789236
C	-3.339402	-1.453515	-3.191419
C	-2.132110	-0.502501	-3.056333
C	-3.779779	-1.482916	-4.664244
C	-4.487747	-0.924951	-2.307990
C	0.472415	-5.460419	1.392141
C	0.947571	-5.662917	-0.064835
C	1.672548	-5.708910	2.322701
C	-0.638448	-6.499132	1.662086
C	-0.429070	-3.200471	3.402489
C	-1.128728	-4.311818	4.207669
C	-1.340223	-1.955644	3.422147
C	0.922062	-2.834532	4.046143
C	-1.841354	1.395388	2.275083
C	-0.393429	1.786549	2.152791
C	0.564535	1.207435	2.945758
C	1.959808	1.468512	2.776568
C	2.248817	2.449029	1.781921
C	1.264048	3.054914	1.046274
C	1.592392	4.154123	0.072289
C	-2.764104	4.026817	3.400090
C	-3.952724	5.006690	3.450863
C	-2.654156	3.246358	4.725749
C	-1.473530	4.861196	3.224464
C	-4.680801	2.126805	1.719001
C	-4.597069	0.905098	0.778509

C	-5.590354	3.179075	1.049886
C	-5.272903	1.665480	3.063796
C	0.866484	5.447648	-2.548799
C	-0.265636	5.521933	-3.596541
C	0.776504	6.689568	-1.633651
C	2.236938	5.474050	-3.250501
C	1.293130	2.314713	-2.273346
C	0.750613	2.194478	-3.711368
C	2.836893	2.287725	-2.265815
C	0.808144	1.073697	-1.489472
H	-1.092788	-4.614960	-3.382596
H	-1.167690	-3.200103	-4.423087
H	1.147362	-2.633425	-4.424082
H	3.048338	-1.732752	-0.668637
H	2.051879	-2.704288	1.308252
H	0.720714	-1.545763	1.274499
H	-2.734874	-5.071416	-4.981228
H	-4.121707	-4.012906	-5.286095
H	-4.372765	-5.721049	-4.931773
H	-5.773815	-3.481308	-3.372926
H	-5.462830	-4.078839	-1.723960
H	-5.954020	-5.199395	-3.004287
H	-2.371086	-6.107186	-2.625338
H	-4.022894	-6.707592	-2.761607
H	-3.553644	-5.770650	-1.337447
H	-1.757181	-0.471717	-2.032612
H	-1.311760	-0.778405	-3.729184
H	-2.449384	0.515181	-3.309884
H	-3.011679	-1.905772	-5.322329
H	-3.963091	-0.452584	-4.995339
H	-4.708138	-2.041554	-4.809368
H	-4.733761	0.099687	-2.614418
H	-5.393047	-1.532109	-2.398347
H	-4.194082	-0.903893	-1.257146
H	0.134445	-5.534858	-0.786275
H	1.760132	-4.985205	-0.343088

H	1.322508	-6.689169	-0.168844
H	2.471631	-4.974530	2.169670
H	2.092891	-6.701459	2.112744
H	1.388576	-5.693350	3.377262
H	-0.244828	-7.503629	1.456404
H	-0.988505	-6.487038	2.695097
H	-1.511610	-6.335004	1.022468
H	-0.492830	-5.190483	4.350636
H	-2.067365	-4.621213	3.735746
H	-1.369183	-3.920950	5.204992
H	-2.350226	-2.187537	3.075005
H	-1.396119	-1.578534	4.452959
H	-0.952779	-1.157622	2.787769
H	0.750376	-2.545148	5.091294
H	1.399433	-1.980257	3.559115
H	1.634830	-3.662015	4.053067
H	-2.068556	0.639040	1.511282
H	-2.056057	0.947296	3.248384
H	0.234561	0.490787	3.688433
H	3.268977	2.790409	1.635949
H	2.666627	4.212886	-0.123439
H	1.276200	5.121684	0.484629
H	-4.060581	5.559542	2.512250
H	-3.770008	5.738524	4.248441
H	-4.899108	4.509280	3.677284
H	-3.507184	2.587963	4.906958
H	-2.607617	3.963570	5.555452
H	-1.738443	2.647176	4.760902
H	-0.577037	4.238537	3.185320
H	-1.378143	5.536790	4.084817
H	-1.513107	5.479723	2.321771
H	-4.086619	1.143926	-0.156892
H	-5.620184	0.592153	0.534089
H	-4.095305	0.045051	1.229740
H	-5.713198	4.085690	1.645863
H	-6.585838	2.740215	0.904251

H	-5.200090	3.470936	0.070599
H	-4.630723	0.928488	3.558638
H	-6.237984	1.179281	2.873698
H	-5.452511	2.493016	3.754905
H	-0.253447	4.674969	-4.287571
H	-0.140053	6.436246	-4.190995
H	-1.249342	5.562610	-3.121233
H	-0.128327	6.695887	-1.020427
H	0.747049	7.585771	-2.265918
H	1.651071	6.780213	-0.980713
H	3.065806	5.390343	-2.539084
H	2.346320	6.434306	-3.770952
H	2.340918	4.684469	-3.998420
H	-0.344613	2.215803	-3.727278
H	1.072120	1.230804	-4.125418
H	1.129204	2.975879	-4.375677
H	3.292943	3.108976	-2.821030
H	3.172170	1.352928	-2.730708
H	3.226885	2.298155	-1.242611
H	1.244607	1.018391	-0.490077
H	1.131812	0.188962	-2.043198
H	-0.275614	1.029441	-1.396424
C	5.318757	-0.029620	3.709556
C	4.998803	-0.678960	4.918001
C	3.701953	-0.587330	5.429870
C	2.712343	0.119146	4.757125
C	2.988716	0.774129	3.529313
C	4.318492	0.693021	3.050698
H	5.743001	-1.280700	5.430044
H	3.459166	-1.083894	6.366316
H	1.720030	0.182584	5.192269
H	4.567507	1.193643	2.121180
C	9.194771	-0.550189	1.908876
C	9.066730	-0.528910	3.297251
C	7.823795	-0.337665	3.899190
C	6.673577	-0.166915	3.110394

C	6.831035	-0.165090	1.717988
C	8.070320	-0.355640	1.088109
H	10.168658	-0.742544	1.469996
H	9.947894	-0.669465	3.917813
H	7.747039	-0.307637	4.981826
H	5.944542	-0.023863	1.112621
C	4.320611	-0.148270	-5.195672
C	5.559476	-0.079279	-4.558836
C	5.765923	-0.723241	-3.326600
C	4.695814	-1.440451	-2.772591
C	3.427909	-1.473837	-3.369252
C	3.255027	-0.825930	-4.605621
H	4.172329	0.365998	-6.141172
H	6.358268	0.509209	-4.999757
H	4.856054	-1.993570	-1.853714
H	2.279811	-0.810759	-5.082077
C	8.278565	-0.410550	-3.226912
C	7.044114	-0.585209	-2.581809
C	7.020945	-0.577425	-1.181336
C	8.166747	-0.375528	-0.398722
C	9.382327	-0.178085	-1.077556
C	9.432930	-0.208076	-2.471262
H	8.339423	-0.446728	-4.310698
H	6.067483	-0.714155	-0.688342
H	10.292237	0.022069	-0.521245
H	10.385499	-0.065203	-2.974419

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C in the closed-shell singlet state SCF = -3548.81987802

Mo	2.408282	-0.085872	-0.029969
Mo	-2.537381	-0.088783	-0.017612
I	3.343016	-2.378550	1.470581
I	-3.287911	-1.502627	-2.392804
P	2.916781	-0.924037	-2.311642
P	3.120394	1.483129	1.705943
P	-2.634427	-2.064192	1.401106

P	-3.194080	2.178674	-0.739902
N	0.526958	0.136612	0.039226
N	-0.676402	0.113317	0.053773
N	2.598689	1.817973	-1.142404
N	-2.891504	0.849432	1.952617
C	3.389689	0.656830	-3.180229
C	2.880369	1.894690	-2.488267
C	2.849373	3.092896	-3.195760
C	2.599124	4.298077	-2.541862
C	2.418264	4.245005	-1.160756
C	2.423861	3.023957	-0.494196
C	2.295214	2.995815	1.002114
C	4.437124	-2.027874	-2.690516
C	4.943551	-1.952403	-4.146367
C	5.574368	-1.536741	-1.763744
C	4.105561	-3.488886	-2.328941
C	1.355897	-1.518146	-3.250475
C	0.433559	-0.293413	-3.421183
C	1.640566	-2.099707	-4.645652
C	0.631394	-2.566163	-2.381261
C	4.982936	1.935097	1.826052
C	5.440269	2.420391	0.431029
C	5.277323	3.052847	2.841727
C	5.801260	0.675270	2.172952
C	2.334723	1.395563	3.458159
C	2.087665	2.775188	4.100313
C	3.194996	0.525846	4.394750
C	0.975935	0.688728	3.276634
C	-1.976108	-1.222792	2.950581
C	-2.512718	0.173486	3.087161
C	-2.599394	0.765560	4.348221
C	-3.079317	2.064565	4.477283
C	-3.503496	2.732549	3.329670
C	-3.424490	2.102759	2.089436
C	-3.993980	2.764317	0.869156
C	-4.478002	-2.451455	1.811255

C	-4.985427	-3.599824	0.916684
C	-4.721855	-2.782574	3.294534
C	-5.313459	-1.197370	1.455174
C	-1.622378	-3.683594	1.354864
C	-0.145317	-3.254909	1.442009
C	-1.826219	-4.367218	-0.014248
C	-1.917328	-4.670209	2.497427
C	-4.676518	2.499643	-1.935021
C	-4.176560	2.349204	-3.385026
C	-5.735554	1.406042	-1.663509
C	-5.385264	3.861825	-1.768700
C	-1.839258	3.503160	-1.032157
C	-0.880744	2.944158	-2.102480
C	-2.303332	4.909792	-1.442190
C	-1.070580	3.630919	0.297588
H	4.485714	0.705527	-3.138508
H	3.121431	0.655793	-4.241654
H	3.055233	3.072596	-4.261901
H	2.573656	5.239662	-3.080897
H	2.267021	5.153063	-0.584320
H	2.627488	3.945455	1.436605
H	1.247260	2.859399	1.283001
H	5.205675	-0.932390	-4.447607
H	4.227581	-2.347107	-4.868151
H	5.857048	-2.556021	-4.230923
H	3.371942	-3.924590	-3.014000
H	3.726917	-3.575385	-1.306356
H	5.019516	-4.093633	-2.400292
H	5.832787	-0.484489	-1.936412
H	6.477637	-2.129708	-1.960407
H	5.319016	-1.659475	-0.708617
H	0.255199	0.210754	-2.473159
H	0.837345	0.435483	-4.132596
H	-0.540732	-0.627027	-3.794570
H	2.193420	-1.398835	-5.281521
H	0.681272	-2.302150	-5.139122

H	2.191258	-3.042933	-4.604562
H	-0.253849	-2.930277	-2.915616
H	1.266090	-3.423573	-2.138955
H	0.281702	-2.124443	-1.446176
H	5.245723	1.670233	-0.341561
H	4.954104	3.353278	0.130625
H	6.522447	2.602983	0.460409
H	4.705789	3.963834	2.630089
H	6.342115	3.316661	2.787723
H	5.071210	2.746626	3.870102
H	6.869770	0.929418	2.158869
H	5.566894	0.273984	3.160336
H	5.630212	-0.126112	1.448907
H	1.380288	3.378579	3.522067
H	3.003633	3.355165	4.231433
H	1.646929	2.628611	5.095629
H	4.133661	1.013696	4.672549
H	2.636809	0.345432	5.323473
H	3.420957	-0.446090	3.945740
H	0.472218	0.620167	4.250351
H	1.118651	-0.320770	2.882427
H	0.303273	1.221114	2.596315
H	-0.900817	-1.161496	2.762646
H	-2.109605	-1.778689	3.885168
H	-2.279094	0.200378	5.217367
H	-3.138348	2.541092	5.451440
H	-3.912748	3.735988	3.387371
H	-3.993325	3.853258	0.982888
H	-5.045232	2.462787	0.792521
H	-4.799120	-3.396037	-0.143500
H	-6.070177	-3.706439	1.052641
H	-4.531222	-4.559635	1.173627
H	-4.151096	-3.651132	3.630755
H	-5.786421	-3.006831	3.447889
H	-4.471821	-1.936063	3.944012
H	-5.091668	-0.346297	2.103607

H	-6.381016	-1.429526	1.572074
H	-5.177742	-0.895306	0.406568
H	0.086069	-2.420527	0.776838
H	0.500764	-4.089138	1.147828
H	0.156512	-2.971133	2.454320
H	-2.842989	-4.733305	-0.167523
H	-1.149821	-5.229994	-0.078941
H	-1.592257	-3.688530	-0.837818
H	-1.800329	-4.204210	3.482807
H	-1.200941	-5.500960	2.444366
H	-2.920589	-5.101123	2.435642
H	-3.501400	3.162712	-3.669898
H	-5.032648	2.379020	-4.072471
H	-3.662002	1.395304	-3.534510
H	-5.351745	0.403141	-1.852193
H	-6.589687	1.565241	-2.335141
H	-6.126132	1.443983	-0.638613
H	-5.754892	4.020766	-0.749703
H	-6.260865	3.883269	-2.431421
H	-4.759169	4.710984	-2.039345
H	-0.408676	2.024106	-1.758570
H	-0.087054	3.671917	-2.303598
H	-1.389859	2.729613	-3.046700
H	-2.730173	4.930635	-2.448268
H	-1.433294	5.581093	-1.448087
H	-3.035009	5.330034	-0.743308
H	-1.654417	4.145538	1.069186
H	-0.162257	4.219172	0.124163
H	-0.776911	2.651387	0.682874

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C in the triplet state SCF = -3548.83343583

Mo	2.519564	-0.097161	-0.055262
Mo	-2.461646	-0.064304	0.008312
I	3.378072	-2.069460	1.883503
I	-3.408253	-1.932039	-1.987895

P	2.716345	-1.453764	-2.122684
P	3.131899	1.783227	1.397314
P	-2.621437	-1.696932	1.831870
P	-3.151743	2.035945	-1.152725
N	0.628825	0.092516	0.029396
N	-0.569335	0.104936	0.056933
N	2.681799	1.521885	-1.537445
N	-2.759332	1.255474	1.743459
C	3.270928	-0.098200	-3.309584
C	2.890767	1.290764	-2.874116
C	2.857896	2.317026	-3.815581
C	2.664592	3.635942	-3.410129
C	2.514161	3.883391	-2.048089
C	2.521071	2.828999	-1.136902
C	2.376008	3.122624	0.332212
C	4.195417	-2.669913	-2.319420
C	4.657552	-2.920462	-3.770719
C	5.384087	-2.047347	-1.549659
C	3.832389	-4.011809	-1.654863
C	1.138618	-2.166957	-2.929679
C	0.227791	-0.968445	-3.261209
C	1.364317	-2.976618	-4.216737
C	0.435052	-3.043461	-1.875321
C	5.002668	2.229919	1.435286
C	5.501822	2.300022	-0.026618
C	5.293027	3.581904	2.110227
C	5.799852	1.112630	2.140250
C	2.329908	2.148328	3.101381
C	2.092583	3.642411	3.395187
C	3.158018	1.509532	4.232551
C	0.968288	1.429105	3.057421
C	-1.878007	-0.578393	3.140829
C	-2.396202	0.822475	3.000861
C	-2.496668	1.643947	4.121564
C	-2.972724	2.946469	3.997924
C	-3.389278	3.370610	2.737303

C	-3.303243	2.512729	1.644155
C	-3.901037	2.924456	0.328206
C	-4.447072	-1.965963	2.393931
C	-5.008139	-3.258067	1.767800
C	-4.604809	-1.999993	3.925638
C	-5.299486	-0.793015	1.854186
C	-1.623375	-3.312084	2.058056
C	-0.134306	-2.915773	2.013372
C	-1.898540	-4.248226	0.862662
C	-1.884738	-4.052514	3.382504
C	-4.648518	2.135737	-2.366148
C	-4.181140	1.660239	-3.755491
C	-5.722793	1.154444	-1.843253
C	-5.320659	3.520617	-2.484910
C	-1.761706	3.228563	-1.716943
C	-0.816926	2.444858	-2.648243
C	-2.220429	4.517780	-2.416454
C	-0.986829	3.623680	-0.446046
H	4.366661	-0.139824	-3.311497
H	2.957802	-0.281316	-4.342594
H	3.005504	2.073400	-4.863003
H	2.644692	4.446401	-4.132314
H	2.385403	4.895878	-1.678009
H	2.722807	4.138843	0.552018
H	1.319351	3.081296	0.606008
H	4.940739	-1.997726	-4.288821
H	3.909088	-3.432001	-4.376089
H	5.549965	-3.560289	-3.748917
H	3.067004	-4.551985	-2.220523
H	3.479467	-3.870557	-0.629118
H	4.724587	-4.651288	-1.616680
H	5.676996	-1.066487	-1.946666
H	6.258416	-2.704844	-1.645896
H	5.170330	-1.941779	-0.483593
H	0.005415	-0.377202	-2.374881
H	0.660915	-0.310925	-4.023830

H	-0.729535	-1.341046	-3.640809
H	1.907236	-2.404682	-4.978211
H	0.386821	-3.241081	-4.640797
H	1.902527	-3.910448	-4.033511
H	-0.514375	-3.409639	-2.281524
H	1.039275	-3.905110	-1.577016
H	0.204797	-2.464938	-0.979458
H	5.324008	1.363168	-0.566395
H	5.035823	3.110591	-0.594807
H	6.584997	2.478667	-0.021943
H	4.730613	4.403335	1.651973
H	6.360615	3.818093	2.006537
H	5.067121	3.565614	3.179495
H	6.872256	1.338149	2.063733
H	5.557234	1.022121	3.200139
H	5.622448	0.135000	1.683272
H	1.406751	4.098797	2.673577
H	3.015093	4.227369	3.405822
H	1.628060	3.740455	4.385696
H	4.092653	2.045929	4.419731
H	2.574066	1.541204	5.162348
H	3.389379	0.460792	4.017581
H	0.428834	1.610674	3.996179
H	1.109619	0.352501	2.933486
H	0.327449	1.775438	2.240726
H	-0.813098	-0.586206	2.897486
H	-1.980017	-0.929861	4.172851
H	-2.186999	1.253356	5.085748
H	-3.039083	3.603195	4.859904
H	-3.805585	4.363009	2.593825
H	-3.897661	4.014501	0.223023
H	-4.954480	2.619122	0.338689
H	-4.868201	-3.271228	0.681495
H	-6.086437	-3.313161	1.968770
H	-4.553558	-4.157519	2.189329
H	-4.015081	-2.789958	4.395620

H	-5.658997	-2.180938	4.175910
H	-4.322372	-1.043791	4.379865
H	-5.002313	0.170460	2.276088
H	-6.350432	-0.963266	2.126251
H	-5.259708	-0.729988	0.759840
H	0.103107	-2.241175	1.189504
H	0.480149	-3.812846	1.878524
H	0.207177	-2.443571	2.938958
H	-2.925468	-4.616591	0.833650
H	-1.234786	-5.119614	0.940211
H	-1.701480	-3.751879	-0.089277
H	-1.724961	-3.406840	4.253770
H	-1.179092	-4.889854	3.464744
H	-2.893464	-4.470534	3.442255
H	-3.474414	2.361963	-4.210813
H	-5.047660	1.587348	-4.426295
H	-3.714459	0.671829	-3.704617
H	-5.348371	0.133171	-1.768021
H	-6.565742	1.145813	-2.546892
H	-6.126143	1.454111	-0.868123
H	-5.617008	3.928447	-1.512301
H	-6.238053	3.412282	-3.078615
H	-4.700080	4.259949	-2.989906
H	-0.313193	1.643072	-2.108213
H	-0.045796	3.117678	-3.040349
H	-1.341865	2.000582	-3.498852
H	-2.660643	4.321640	-3.397534
H	-1.345545	5.163026	-2.575512
H	-2.941125	5.085588	-1.818148
H	-1.563433	4.289082	0.204878
H	-0.076334	4.157190	-0.742182
H	-0.699951	2.740211	0.130364

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C in the quintet state SCF = -3548.82241780

Mo 2.498806 -0.145038 -0.049253

Mo	-2.546010	-0.005874	-0.005573
I	3.081907	-1.891222	2.157356
I	-3.492411	-1.984048	-1.908925
P	2.699162	-1.791140	-1.958033
P	3.347142	1.866227	1.203970
P	-2.781373	-1.467586	1.936928
P	-3.023779	2.046937	-1.321400
N	0.526503	-0.022388	0.115938
N	-0.665888	0.021247	0.083406
N	2.881259	1.273926	-1.695917
N	-2.718955	1.468956	1.621402
C	3.340524	-0.598406	-3.249863
C	3.016585	0.853605	-3.000220
C	3.001997	1.748150	-4.063778
C	2.910951	3.121720	-3.830303
C	2.853919	3.553703	-2.503731
C	2.835666	2.630898	-1.465481
C	2.747279	3.116852	-0.038624
C	4.096552	-3.105144	-1.915043
C	4.585490	-3.551382	-3.308984
C	5.295312	-2.478808	-1.167434
C	3.606208	-4.330803	-1.119265
C	1.091695	-2.504170	-2.704850
C	0.270726	-1.291533	-3.187151
C	1.286230	-3.470436	-3.884619
C	0.307215	-3.201645	-1.574929
C	5.245582	2.131471	1.271869
C	5.765839	2.112912	-0.183414
C	5.670093	3.463632	1.914973
C	5.890059	0.944630	2.016222
C	2.509760	2.448505	2.826024
C	2.439210	3.982309	2.970584
C	3.229687	1.838252	4.044490
C	1.071681	1.890164	2.797860
C	-1.933372	-0.301738	3.145461
C	-2.358697	1.116211	2.903559

C	-2.379376	2.032539	3.952753
C	-2.769852	3.350528	3.727040
C	-3.179766	3.698461	2.441279
C	-3.173452	2.748866	1.422651
C	-3.742913	3.090336	0.075596
C	-4.622424	-1.541360	2.505184
C	-5.280142	-2.839246	1.996728
C	-4.793268	-1.411802	4.030480
C	-5.376527	-0.365469	1.837768
C	-1.917502	-3.133374	2.314446
C	-0.401006	-2.860818	2.268719
C	-2.245595	-4.137051	1.189441
C	-2.256114	-3.736176	3.689221
C	-4.486096	2.157725	-2.573155
C	-4.016443	1.562082	-3.914016
C	-5.620890	1.268700	-2.014030
C	-5.077950	3.565712	-2.796300
C	-1.548199	3.108335	-1.928644
C	-0.641353	2.209338	-2.790036
C	-1.909533	4.380216	-2.712496
C	-0.756019	3.527656	-0.674947
H	4.434079	-0.682808	-3.201971
H	3.048342	-0.892401	-4.262824
H	3.096008	1.362806	-5.074361
H	2.905261	3.830573	-4.652006
H	2.812590	4.612206	-2.264965
H	3.232119	4.094725	0.057635
H	1.693926	3.256672	0.220676
H	4.973762	-2.716700	-3.903111
H	3.813721	-4.054121	-3.891817
H	5.412386	-4.261899	-3.178651
H	2.831654	-4.885435	-1.657405
H	3.218198	-4.045731	-0.136489
H	4.449361	-5.015562	-0.959299
H	5.679564	-1.582760	-1.670118
H	6.112874	-3.211677	-1.136686

H	5.039846	-2.209755	-0.140080
H	0.127925	-0.569152	-2.384431
H	0.733153	-0.783446	-4.041323
H	-0.727381	-1.626928	-3.489146
H	1.880607	-3.029776	-4.693992
H	0.300766	-3.718106	-4.299708
H	1.756074	-4.410086	-3.580483
H	-0.642657	-3.574119	-1.974105
H	0.852518	-4.044563	-1.141720
H	0.064830	-2.499587	-0.775448
H	5.460775	1.203276	-0.711328
H	5.422164	2.976618	-0.761920
H	6.862824	2.142456	-0.164876
H	5.217262	4.327225	1.413603
H	6.759509	3.572720	1.828387
H	5.423642	3.513431	2.978467
H	6.982547	1.054559	1.987216
H	5.589098	0.885926	3.064312
H	5.624465	-0.007156	1.546697
H	1.851364	4.444628	2.170527
H	3.422216	4.457694	2.991684
H	1.938570	4.224453	3.917308
H	4.227144	2.259648	4.196146
H	2.642421	2.056515	4.946240
H	3.316729	0.750931	3.957244
H	0.537688	2.232757	3.693410
H	1.072112	0.797613	2.787109
H	0.500528	2.228536	1.928674
H	-0.875808	-0.400327	2.882339
H	-2.034117	-0.565289	4.204006
H	-2.077867	1.702835	4.942042
H	-2.774642	4.078793	4.532320
H	-3.526775	4.703321	2.220496
H	-3.683412	4.167784	-0.111490
H	-4.809767	2.836387	0.092931
H	-5.151137	-2.956111	0.915083

H	-6.358142	-2.799432	2.203767
H	-4.887778	-3.729753	2.492401
H	-4.282332	-2.203941	4.582312
H	-5.860914	-1.469606	4.283514
H	-4.423980	-0.447002	4.395688
H	-5.022921	0.609614	2.181259
H	-6.444094	-0.438036	2.087653
H	-5.306106	-0.402944	0.742170
H	-0.099639	-2.273625	1.399451
H	0.138846	-3.813695	2.218799
H	-0.036500	-2.343852	3.160388
H	-3.302702	-4.404843	1.142724
H	-1.676373	-5.059970	1.365139
H	-1.963814	-3.741824	0.210977
H	-2.052884	-3.034121	4.506016
H	-1.623743	-4.618658	3.855166
H	-3.296466	-4.062995	3.765337
H	-3.264286	2.192235	-4.400311
H	-4.870879	1.483527	-4.599504
H	-3.603044	0.557854	-3.777306
H	-5.303884	0.233445	-1.878883
H	-6.454599	1.267795	-2.728786
H	-6.018744	1.642331	-1.062248
H	-5.392409	4.039413	-1.859723
H	-5.973850	3.472965	-3.424691
H	-4.396755	4.244606	-3.308436
H	-0.234345	1.391700	-2.194955
H	0.200992	2.796450	-3.174270
H	-1.168473	1.775780	-3.644801
H	-2.357158	4.153844	-3.683747
H	-0.990819	4.952097	-2.903724
H	-2.592563	5.033062	-2.157893
H	-1.303510	4.237537	-0.046344
H	0.166619	4.022272	-1.002210
H	-0.488827	2.660132	-0.065905

TSC/PC in the closed-shell singlet state SCF = -3548.79820293

Mo	2.470918	-0.087423	-0.065415
Mo	-2.449423	-0.085840	0.006945
I	3.515264	-1.917535	1.967204
I	-3.538565	-1.944465	-1.945925
P	2.825471	-1.496718	-2.066859
P	3.259073	1.910165	1.220264
P	-2.579539	-1.702522	1.857754
P	-3.426607	1.987988	-1.053034
N	0.758585	-0.088760	0.210788
N	-0.738564	-0.024238	-0.247599
N	2.627885	1.467783	-1.637417
N	-2.716532	1.233568	1.788126
C	3.337803	-0.187145	-3.311427
C	2.830683	1.182857	-2.963790
C	2.672550	2.142245	-3.958053
C	2.359073	3.458523	-3.616795
C	2.252500	3.774302	-2.265950
C	2.396298	2.779024	-1.299401
C	2.334737	3.148158	0.159974
C	4.314964	-2.700637	-2.209135
C	4.773570	-3.001937	-3.651544
C	5.497555	-2.036648	-1.467244
C	3.958252	-4.016620	-1.491183
C	1.248536	-2.244852	-2.848563
C	0.348114	-1.049009	-3.227321
C	1.481985	-3.097508	-4.106248
C	0.527965	-3.085901	-1.779136
C	5.100249	2.413852	1.085154
C	5.465045	2.496130	-0.414710
C	5.416400	3.772786	1.733032
C	5.967444	1.303296	1.714469
C	2.558000	2.278519	2.962882
C	2.305842	3.777594	3.223595
C	3.493675	1.702887	4.043892

C	1.212073	1.529952	3.053510
C	-1.720574	-0.596581	3.102325
C	-2.229291	0.810429	3.002513
C	-2.193571	1.647644	4.115915
C	-2.665242	2.954243	4.024225
C	-3.213262	3.367845	2.811985
C	-3.256304	2.492301	1.729339
C	-3.996227	2.896657	0.483828
C	-4.364261	-1.968879	2.541355
C	-4.970697	-3.247076	1.927092
C	-4.410850	-2.027864	4.079674
C	-5.251495	-0.788032	2.083835
C	-1.571534	-3.323636	2.003215
C	-0.078751	-2.938336	1.938939
C	-1.893713	-4.223236	0.792731
C	-1.797897	-4.100198	3.314482
C	-5.025875	2.062424	-2.112839
C	-4.685458	1.612053	-3.545939
C	-6.009785	1.044197	-1.491551
C	-5.730946	3.434227	-2.141743
C	-2.064381	3.125033	-1.769043
C	-1.288258	2.352509	-2.854661
C	-2.582209	4.450405	-2.352378
C	-1.093457	3.451216	-0.614896
H	4.433192	-0.141187	-3.260396
H	3.083705	-0.452451	-4.342400
H	2.815129	1.854929	-4.994827
H	2.231741	4.218884	-4.381291
H	2.058101	4.793685	-1.946967
H	2.640257	4.191738	0.300074
H	1.303627	3.064904	0.518617
H	5.037343	-2.094838	-4.206416
H	4.030428	-3.550181	-4.230817
H	5.677034	-3.624810	-3.608959
H	3.188587	-4.577789	-2.030216
H	3.613450	-3.836751	-0.468480

H	4.851782	-4.652889	-1.436095
H	5.789702	-1.078860	-1.916620
H	6.371699	-2.699188	-1.523100
H	5.272922	-1.868985	-0.412030
H	0.219415	-0.367480	-2.387205
H	0.742217	-0.491336	-4.084766
H	-0.649596	-1.418249	-3.491425
H	2.037462	-2.557852	-4.882032
H	0.505391	-3.364662	-4.530549
H	2.007977	-4.030883	-3.886524
H	-0.418138	-3.456353	-2.191241
H	1.122377	-3.944642	-1.452136
H	0.291343	-2.480357	-0.905302
H	5.253816	1.558420	-0.938697
H	4.936837	3.302990	-0.931837
H	6.541076	2.694064	-0.501951
H	4.797621	4.578587	1.321288
H	6.465317	4.031979	1.536389
H	5.283943	3.755420	2.817482
H	7.026727	1.542537	1.550120
H	5.813150	1.201943	2.790000
H	5.759442	0.327949	1.264534
H	1.551822	4.191318	2.545736
H	3.209972	4.384980	3.141270
H	1.921225	3.898319	4.244958
H	4.425574	2.269061	4.133281
H	2.985727	1.758323	5.015959
H	3.732732	0.652258	3.850097
H	0.744279	1.760438	4.019470
H	1.358915	0.449907	2.981204
H	0.508439	1.819147	2.266843
H	-0.676942	-0.610819	2.772625
H	-1.743216	-0.947574	4.139654
H	-1.783355	1.266485	5.045341
H	-2.627596	3.623872	4.878091
H	-3.632270	4.363211	2.701483

H	-3.990248	3.985146	0.364819
H	-5.045345	2.605844	0.620006
H	-4.917548	-3.228718	0.832962
H	-6.029774	-3.310129	2.210834
H	-4.485009	-4.157921	2.283617
H	-3.796499	-2.829146	4.493589
H	-5.445569	-2.203832	4.403563
H	-4.086693	-1.081328	4.527098
H	-4.920321	0.169092	2.495232
H	-6.277957	-0.963205	2.434024
H	-5.284798	-0.707524	0.991859
H	0.146930	-2.207304	1.162510
H	0.517565	-3.833125	1.727127
H	0.291031	-2.536523	2.886984
H	-2.935495	-4.548516	0.764890
H	-1.264420	-5.121639	0.847097
H	-1.685000	-3.716280	-0.150283
H	-1.605644	-3.481067	4.198061
H	-1.089761	-4.938553	3.347930
H	-2.803215	-4.521313	3.397426
H	-4.081280	2.357018	-4.073741
H	-5.614933	1.481396	-4.115699
H	-4.153874	0.655234	-3.549941
H	-5.603311	0.031449	-1.491808
H	-6.932113	1.034936	-2.087068
H	-6.293644	1.307939	-0.465222
H	-5.980673	3.797073	-1.138750
H	-6.677832	3.327603	-2.687532
H	-5.153164	4.206763	-2.649684
H	-0.861136	1.433932	-2.450658
H	-0.464263	2.976249	-3.223116
H	-1.918238	2.087606	-3.708332
H	-3.161919	4.302087	-3.267099
H	-1.721374	5.080292	-2.613592
H	-3.194734	5.013308	-1.639528
H	-1.559193	4.062392	0.166037

H	-0.251437	4.022242	-1.022434
H	-0.698591	2.538925	-0.161136

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TSC/PC in the triplet state SCF = -3548.77320571

Mo	2.435532	-0.076829	-0.088344
Mo	-2.458834	-0.082916	0.009899
I	3.450214	-2.095112	1.785452
I	-3.643586	-1.661240	-2.072008
P	2.756044	-1.317196	-2.228688
P	3.276632	1.788306	1.351822
P	-2.494822	-1.963940	1.675938
P	-3.423582	2.173337	-0.783771
N	0.731612	-0.052280	0.191155
N	-0.799493	0.086082	-0.462854
N	2.614584	1.596586	-1.509432
N	-2.548976	1.000023	1.891476
C	3.337837	0.094390	-3.317775
C	2.826468	1.430759	-2.861162
C	2.678209	2.470622	-3.768160
C	2.372178	3.759565	-3.320196
C	2.273628	3.957713	-1.943277
C	2.404753	2.885829	-1.064861
C	2.361884	3.129121	0.421195
C	4.200636	-2.558507	-2.455967
C	4.670800	-2.760560	-3.911431
C	5.400842	-2.004606	-1.653145
C	3.778035	-3.908143	-1.844594
C	1.170757	-1.914355	-3.121747
C	0.335529	-0.653138	-3.434525
C	1.416043	-2.670060	-4.438153
C	0.364763	-2.802801	-2.157923
C	5.130288	2.253143	1.217651
C	5.475478	2.453599	-0.275571
C	5.489024	3.546263	1.970397
C	5.984495	1.078306	1.739019

C	2.634263	2.024125	3.137707
C	2.421616	3.501576	3.526159
C	3.581148	1.341320	4.143948
C	1.275058	1.299729	3.202825
C	-1.524294	-0.986179	2.929566
C	-2.043542	0.415176	3.052158
C	-1.962505	1.094079	4.253890
C	-2.361987	2.434176	4.352781
C	-2.913296	3.016389	3.203377
C	-3.029511	2.298254	2.025319
C	-3.840864	2.870164	0.891752
C	-4.249931	-2.246748	2.414386
C	-4.935191	-3.432531	1.706128
C	-4.203978	-2.470668	3.938777
C	-5.117696	-0.996064	2.141960
C	-1.536875	-3.610841	1.562037
C	-0.039363	-3.256066	1.459320
C	-1.956543	-4.355585	0.278808
C	-1.718948	-4.523718	2.789340
C	-5.093428	2.352570	-1.697287
C	-4.883130	2.078889	-3.199352
C	-6.042055	1.277782	-1.117862
C	-5.773053	3.726451	-1.508690
C	-2.087715	3.344875	-1.480656
C	-1.423394	2.684555	-2.705809
C	-2.614288	4.739265	-1.862217
C	-1.025544	3.510287	-0.373832
H	4.430768	0.114362	-3.214650
H	3.125999	-0.069976	-4.378731
H	2.827263	2.270792	-4.824779
H	2.253033	4.582996	-4.017133
H	2.097141	4.949147	-1.536515
H	2.689699	4.150082	0.649420
H	1.334526	3.030400	0.787831
H	4.954410	-1.818090	-4.393037
H	3.927720	-3.253121	-4.538594

H	5.564461	-3.398803	-3.905473
H	2.992301	-4.392818	-2.433056
H	3.425851	-3.786402	-0.815612
H	4.641461	-4.586503	-1.825754
H	5.753136	-1.039488	-2.038705
H	6.239056	-2.709161	-1.737080
H	5.170158	-1.893136	-0.591961
H	0.225116	-0.018397	-2.555541
H	0.763880	-0.065239	-4.253668
H	-0.674624	-0.962166	-3.730292
H	2.039693	-2.102847	-5.138189
H	0.446629	-2.837286	-4.925596
H	1.872643	-3.650680	-4.278091
H	-0.537610	-3.159849	-2.668950
H	0.929536	-3.672989	-1.810168
H	0.040183	-2.227450	-1.292352
H	5.239751	1.567409	-0.872846
H	4.954187	3.308305	-0.716620
H	6.553750	2.639658	-0.362391
H	4.880754	4.396284	1.640854
H	6.539585	3.798574	1.773838
H	5.376822	3.440727	3.052011
H	7.045346	1.309513	1.573045
H	5.848118	0.894012	2.805749
H	5.749743	0.145951	1.217421
H	1.655926	3.981810	2.908064
H	3.334950	4.097372	3.465770
H	2.068397	3.544289	4.564796
H	4.527833	1.877495	4.259227
H	3.094732	1.326149	5.128298
H	3.791116	0.305592	3.858410
H	0.837937	1.460307	4.195714
H	1.396242	0.226436	3.038551
H	0.556250	1.667923	2.464596
H	-0.516324	-0.945943	2.494983
H	-1.447252	-1.471185	3.907276

H	-1.550443	0.573430	5.113249
H	-2.276707	2.985150	5.282794
H	-3.301022	4.031233	3.231114
H	-3.807030	3.964513	0.897335
H	-4.889495	2.590340	1.059744
H	-4.950284	-3.294366	0.619367
H	-5.975889	-3.496863	2.050177
H	-4.460499	-4.390344	1.928587
H	-3.607087	-3.338316	4.226900
H	-5.225278	-2.637682	4.306600
H	-3.808604	-1.591025	4.458390
H	-4.717836	-0.097124	2.616122
H	-6.122138	-1.174209	2.549825
H	-5.229709	-0.806583	1.068666
H	0.170563	-2.452282	0.753370
H	0.516450	-4.140492	1.126829
H	0.386139	-2.962693	2.422166
H	-3.005600	-4.659385	0.283532
H	-1.346277	-5.263375	0.186197
H	-1.793249	-3.742962	-0.609107
H	-1.451407	-4.014880	3.721938
H	-1.043096	-5.382143	2.683670
H	-2.733744	-4.917862	2.885463
H	-4.309382	2.876502	-3.681928
H	-5.860901	2.032831	-3.696067
H	-4.375581	1.125273	-3.372243
H	-5.654676	0.267248	-1.258653
H	-7.006106	1.341920	-1.638869
H	-6.242290	1.428827	-0.050602
H	-5.945436	3.967016	-0.454293
H	-6.756331	3.695209	-1.995719
H	-5.215056	4.547268	-1.960109
H	-1.017662	1.703739	-2.452826
H	-0.591518	3.313902	-3.046418
H	-2.119114	2.564301	-3.541598
H	-3.274814	4.708688	-2.732763

H	-1.759877	5.376442	-2.125362
H	-3.145160	5.228684	-1.037867
H	-1.416131	4.023964	0.510782
H	-0.203078	4.111684	-0.775870
H	-0.615294	2.545418	-0.068228

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PC (2×B) in the closed-shell singlet state SCF = -3548.86565467

Mo	-4.381830	-0.186003	-0.688845
Mo	3.787389	0.099853	-0.000210
I	-6.213216	-2.445627	-0.507326
I	2.343627	0.300525	2.499555
P	-2.233980	-1.455728	-0.861871
P	-5.884583	1.384741	0.498844
P	4.805444	-2.099739	0.535565
P	3.950750	2.544677	-0.573151
N	-4.620025	0.433340	-2.207977
N	2.705899	-0.490467	-1.111632
N	-2.921513	1.339938	0.066115
N	5.725879	0.169810	-1.177236
C	-1.114064	-0.348194	0.167774
C	-1.596027	1.074836	0.253905
C	-0.687010	2.081381	0.578800
C	-1.134807	3.389751	0.730373
C	-2.489529	3.657862	0.561742
C	-3.367502	2.621820	0.242125
C	-4.844221	2.908952	0.122178
C	-1.947717	-3.136233	0.005658
C	-0.475233	-3.449181	0.327789
C	-2.726294	-3.067755	1.340816
C	-2.552465	-4.257926	-0.859060
C	-1.471056	-1.405606	-2.615304
C	-1.265687	0.080516	-2.982258
C	-0.115880	-2.125867	-2.726659
C	-2.481012	-2.024874	-3.604031
C	-5.916820	1.267977	2.410904

C	-4.461409	1.310713	2.930126
C	-6.698171	2.405020	3.092665
C	-6.511754	-0.098869	2.814283
C	-7.599403	1.870761	-0.195351
C	-7.983819	3.341354	0.067621
C	-8.674825	0.926728	0.378101
C	-7.541557	1.645195	-1.722399
C	5.645330	-2.290912	-1.138483
C	6.302477	-1.011302	-1.562765
C	7.464678	-1.041811	-2.334270
C	8.061818	0.149254	-2.733544
C	7.485469	1.348941	-2.327987
C	6.332788	1.334925	-1.542049
C	5.772171	2.634191	-1.034148
C	6.234816	-2.011848	1.809017
C	5.710707	-2.408565	3.204167
C	7.450189	-2.874997	1.421927
C	6.695663	-0.536442	1.897186
C	3.829195	-3.737002	0.678770
C	3.011424	-3.905183	-0.621738
C	2.834320	-3.618645	1.851644
C	4.724388	-4.977072	0.855754
C	3.875720	3.985979	0.694987
C	2.400009	4.244530	1.046341
C	4.598439	3.485173	1.967289
C	4.553321	5.300147	0.254486
C	3.051792	2.970128	-2.212911
C	1.555817	2.637979	-2.057488
C	3.211424	4.436855	-2.646327
C	3.640709	2.063902	-3.318301
H	-1.127530	-0.757860	1.184345
H	-0.065690	-0.381776	-0.146538
H	0.352458	1.816138	0.727943
H	-0.441792	4.183236	0.992439
H	-2.879302	4.662738	0.689871
H	-5.104395	3.798698	0.707577

H	-5.086023	3.123227	-0.926054
H	-0.006027	-2.676483	0.944113
H	0.133233	-3.579558	-0.565851
H	-0.428215	-4.387996	0.896912
H	-1.973639	-4.422083	-1.773495
H	-3.590741	-4.042088	-1.130208
H	-2.542119	-5.197605	-0.290655
H	-2.356488	-2.272711	2.000859
H	-2.593691	-4.015771	1.878786
H	-3.797887	-2.924055	1.181361
H	-2.199945	0.644921	-2.922987
H	-0.516065	0.558979	-2.345019
H	-0.897709	0.137452	-4.015440
H	0.628563	-1.734832	-2.026138
H	0.281101	-1.967137	-3.738845
H	-0.210550	-3.206388	-2.585424
H	-2.082739	-1.930203	-4.623590
H	-2.650040	-3.088009	-3.411099
H	-3.445729	-1.512778	-3.559984
H	-3.841166	0.519728	2.497382
H	-3.972244	2.269758	2.736321
H	-4.473647	1.160043	4.017176
H	-6.324672	3.394312	2.803795
H	-6.587375	2.317242	4.181784
H	-7.767240	2.362643	2.870874
H	-6.446318	-0.207745	3.905538
H	-7.560688	-0.205009	2.532668
H	-5.969769	-0.929699	2.352379
H	-7.284126	4.037791	-0.406970
H	-8.044321	3.588662	1.129546
H	-8.973007	3.530768	-0.369660
H	-8.874172	1.113312	1.437618
H	-9.615332	1.093548	-0.163191
H	-8.395441	-0.124281	0.247728
H	-8.506637	1.944876	-2.152911
H	-7.356419	0.597124	-1.967607

H	-6.757868	2.235018	-2.207969
H	4.808715	-2.486316	-1.817156
H	6.342011	-3.132047	-1.214130
H	7.885984	-1.999988	-2.619494
H	8.961819	0.143052	-3.341273
H	7.925027	2.300985	-2.606985
H	5.987715	3.443669	-1.739191
H	6.298262	2.885878	-0.105836
H	4.823190	-1.828685	3.480294
H	6.491589	-2.202958	3.947770
H	5.469378	-3.471992	3.272170
H	7.202074	-3.933454	1.314468
H	8.214850	-2.793183	2.205414
H	7.905632	-2.531352	0.486311
H	7.110267	-0.170159	0.954028
H	7.484352	-0.456522	2.656882
H	5.877933	0.125218	2.208639
H	2.461803	-2.997104	-0.882843
H	2.284105	-4.711413	-0.471829
H	3.638131	-4.194143	-1.472380
H	3.328062	-3.548534	2.822478
H	2.196909	-4.511775	1.866639
H	2.193423	-2.741495	1.741954
H	5.455286	-5.078384	0.045155
H	4.093534	-5.875239	0.839695
H	5.262620	-4.975697	1.807150
H	1.841995	4.644193	0.193730
H	2.341125	4.983828	1.855881
H	1.913706	3.329209	1.396543
H	4.152008	2.569586	2.360731
H	4.517695	4.255411	2.745188
H	5.669326	3.312515	1.803229
H	5.602456	5.156133	-0.025326
H	4.542070	5.999095	1.101126
H	4.044119	5.790841	-0.575286
H	1.414670	1.594842	-1.768115

H	1.047508	2.795653	-3.017462
H	1.060632	3.270697	-1.317139
H	2.681887	5.122185	-1.979409
H	2.777919	4.558994	-3.647148
H	4.260325	4.748527	-2.704361
H	4.689127	2.298608	-3.534077
H	3.073671	2.232164	-4.242720
H	3.558661	1.004571	-3.062419

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PC (2×B) in the triplet state SCF = -3548.83044817

Mo	-4.354090	-0.181517	-0.734317
Mo	3.778082	0.099815	-0.007525
I	-6.139938	-2.397796	-0.510753
I	2.242026	0.225465	2.440057
P	-2.123790	-1.436746	-0.881565
P	-5.935075	1.379378	0.537553
P	4.818710	-2.089583	0.520625
P	3.932177	2.561459	-0.517194
N	-4.592021	0.334472	-2.294424
N	2.739488	-0.479294	-1.166398
N	-3.011216	1.302650	0.093255
N	5.753049	0.220900	-1.111383
C	-1.097163	-0.294160	0.160180
C	-1.617171	1.117158	0.180855
C	-0.739860	2.152248	0.408267
C	-1.193237	3.475550	0.575985
C	-2.586751	3.673523	0.510722
C	-3.449297	2.628664	0.269412
C	-4.933542	2.897454	0.178808
C	-1.897880	-3.111611	0.000447
C	-0.421962	-3.394601	0.343004
C	-2.688919	-3.047100	1.328079
C	-2.468575	-4.248029	-0.867235
C	-1.383501	-1.408219	-2.638428
C	-1.206975	0.079463	-3.018896

C	-0.014910	-2.105080	-2.736271
C	-2.380605	-2.060133	-3.618482
C	-5.975789	1.192134	2.438450
C	-4.527272	1.307426	2.966158
C	-6.825217	2.279299	3.122670
C	-6.505797	-0.207846	2.813018
C	-7.656139	1.767669	-0.188855
C	-8.091735	3.224005	0.078847
C	-8.709784	0.791149	0.368923
C	-7.566038	1.555575	-1.716431
C	5.707846	-2.240957	-1.131878
C	6.361882	-0.943772	-1.505671
C	7.551205	-0.941070	-2.232868
C	8.150036	0.266851	-2.580684
C	7.542639	1.449046	-2.164638
C	6.362630	1.402428	-1.423797
C	5.769612	2.680391	-0.900004
C	6.211638	-2.000602	1.834695
C	5.660019	-2.436197	3.207258
C	7.451871	-2.833954	1.461618
C	6.642834	-0.519412	1.967310
C	3.868844	-3.747124	0.614699
C	3.076930	-3.897730	-0.704205
C	2.852952	-3.670625	1.772676
C	4.779092	-4.977524	0.781032
C	3.789519	3.972590	0.779932
C	2.298993	4.210794	1.074290
C	4.465309	3.456225	2.071563
C	4.470930	5.301267	0.391465
C	3.098634	3.015714	-2.184716
C	1.600887	2.666164	-2.106873
C	3.259231	4.494038	-2.578005
C	3.748469	2.142619	-3.282870
H	-1.147801	-0.701908	1.178329
H	-0.040698	-0.323129	-0.123792
H	0.312026	1.906562	0.500430

H	-0.512647	4.292154	0.782084
H	-3.008330	4.666259	0.650482
H	-5.214205	3.747713	0.809755
H	-5.205887	3.155669	-0.853558
H	0.020175	-2.610275	0.963650
H	0.202828	-3.515154	-0.540781
H	-0.368050	-4.330880	0.914375
H	-1.868279	-4.411978	-1.767090
H	-3.503765	-4.053472	-1.164125
H	-2.455593	-5.181073	-0.288968
H	-2.336892	-2.244294	1.985755
H	-2.543631	-3.992351	1.867174
H	-3.761312	-2.922087	1.164225
H	-2.151552	0.628493	-2.982411
H	-0.483806	0.585121	-2.374220
H	-0.826985	0.128718	-4.047857
H	0.721178	-1.687570	-2.042768
H	0.378553	-1.953179	-3.750401
H	-0.089642	-3.185379	-2.579853
H	-1.988781	-1.955205	-4.638883
H	-2.516761	-3.127991	-3.425603
H	-3.359896	-1.575336	-3.579142
H	-3.863295	0.563551	2.517560
H	-4.089951	2.292314	2.782027
H	-4.541892	1.139964	4.050661
H	-6.496041	3.289716	2.855286
H	-6.720305	2.178965	4.210772
H	-7.888922	2.187495	2.888842
H	-6.467860	-0.318724	3.904862
H	-7.537625	-0.374063	2.497607
H	-5.897152	-1.001153	2.369931
H	-7.411164	3.946391	-0.383313
H	-8.170863	3.459770	1.141972
H	-9.082408	3.381087	-0.367087
H	-8.918689	0.962720	1.428659
H	-9.650214	0.940424	-0.176939

H	-8.406717	-0.251723	0.232784
H	-8.529492	1.836047	-2.162174
H	-7.357251	0.513672	-1.969471
H	-6.789113	2.168630	-2.183634
H	4.893719	-2.432443	-1.838350
H	6.417819	-3.071524	-1.203369
H	7.994723	-1.887320	-2.524822
H	9.071972	0.286612	-3.153978
H	7.980983	2.413420	-2.400409
H	6.005122	3.513637	-1.570216
H	6.253662	2.908699	0.057047
H	4.754141	-1.879536	3.471530
H	6.417118	-2.230566	3.975158
H	5.439168	-3.505578	3.247782
H	7.224329	-3.893703	1.324152
H	8.194213	-2.757109	2.266892
H	7.924910	-2.461652	0.546101
H	7.080934	-0.126231	1.046102
H	7.404958	-0.442240	2.754040
H	5.803755	0.121470	2.265127
H	2.525898	-2.988370	-0.958098
H	2.355411	-4.715016	-0.586387
H	3.723577	-4.161216	-1.548174
H	3.329915	-3.630407	2.753384
H	2.219847	-4.567035	1.749277
H	2.210824	-2.792214	1.682561
H	5.525514	-5.050485	-0.018217
H	4.162792	-5.885037	0.735367
H	5.300870	-4.987674	1.741609
H	1.770363	4.614675	0.205834
H	2.199061	4.939318	1.889573
H	1.804471	3.288925	1.392611
H	4.005849	2.535894	2.437527
H	4.352285	4.217224	2.854654
H	5.542321	3.287492	1.947409
H	5.532772	5.174010	0.153939

H	4.415008	5.985160	1.248641
H	3.991053	5.800430	-0.450532
H	1.456045	1.620000	-1.830989
H	1.142519	2.824035	-3.091995
H	1.056964	3.287742	-1.392130
H	2.693270	5.156873	-1.918441
H	2.865325	4.633524	-3.592966
H	4.305692	4.819355	-2.585522
H	4.802534	2.393999	-3.446566
H	3.220644	2.325582	-4.227647
H	3.669286	1.076857	-3.054393