Supplementary Information for

Bis-ketopyrrolyl complexes of Co(II) stabilised by trimethylphosphine ligands

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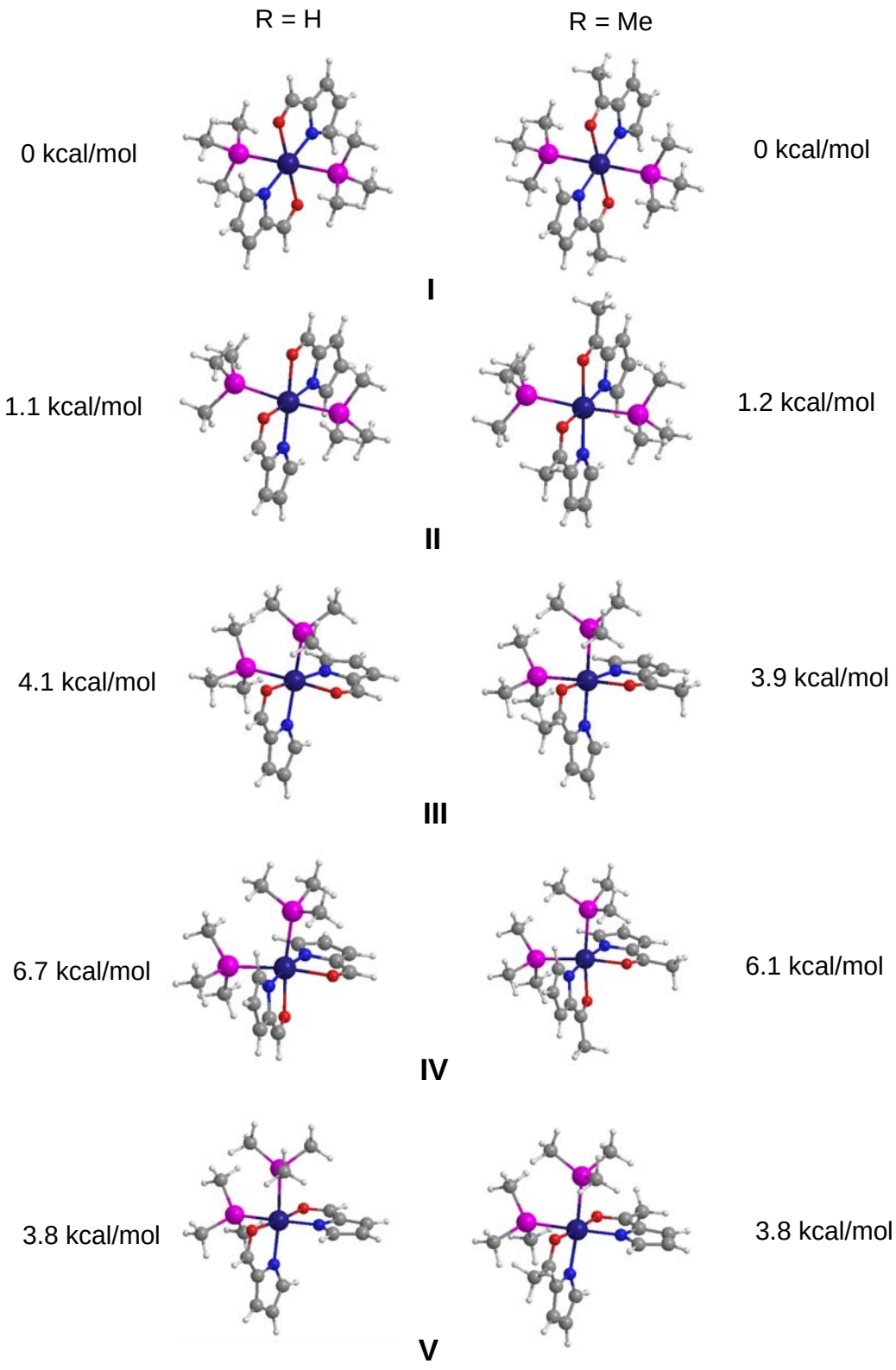

Fig. S1. Optimised geometries and relative energy (B3LYP/b1) of the *S*=3/2 [Co(2-ketopyrrolyl)$_2$(PMe$_3$)$_2$] complexes with 2-formylpyrrolyl (left) and 2-acetylpyrrolyl (right) ligands.

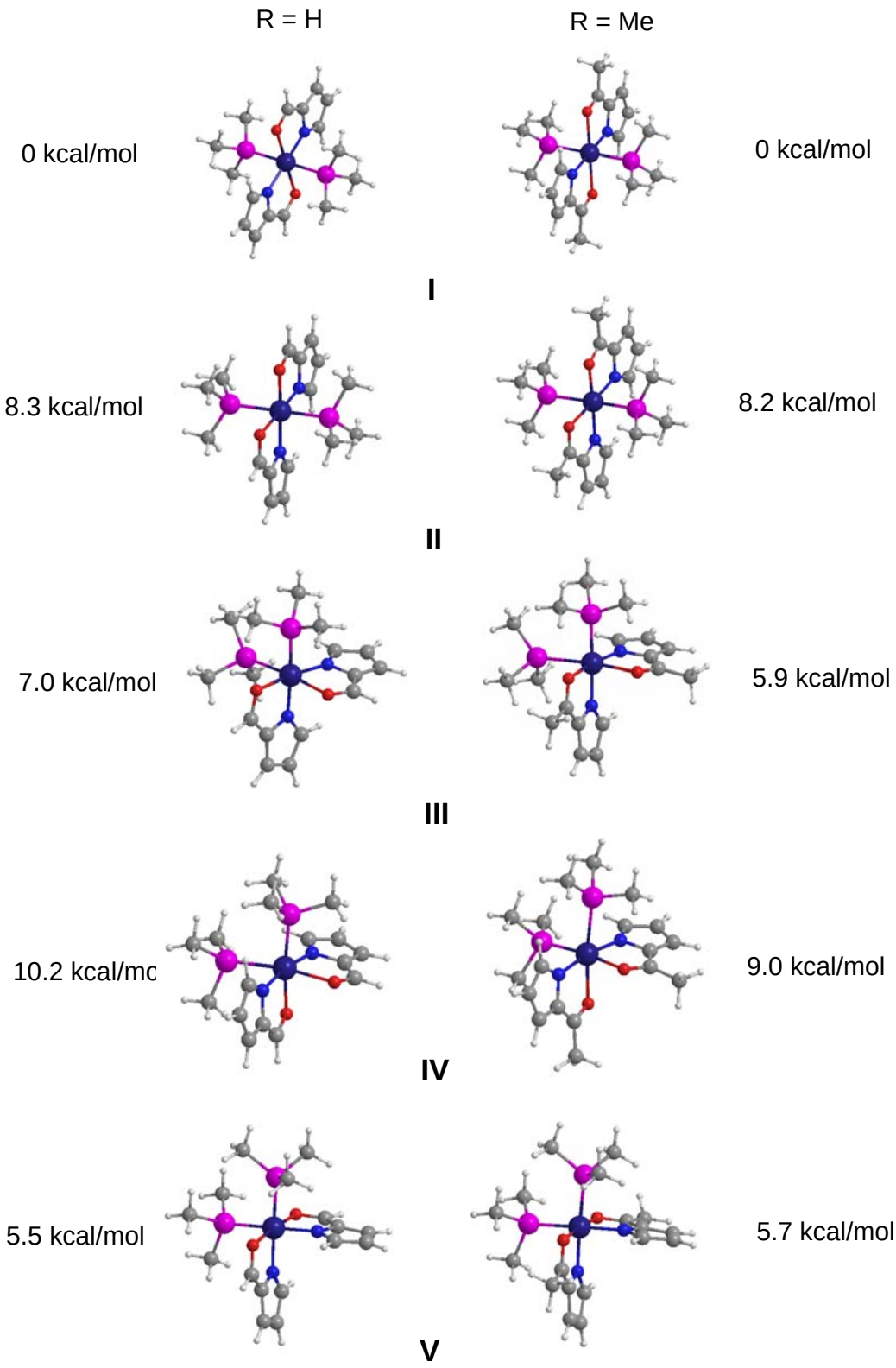

Fig. S2. Optimised geometries and relative energy (B3LYP/b1) of the *S*=1/2 [Co(2-ketopyrrolyl)$_2$(PMe$_3$)$_2$] complexes with 2-formylpyrrolyl (left) and 2-acetylpyrrolyl (right) ligands.

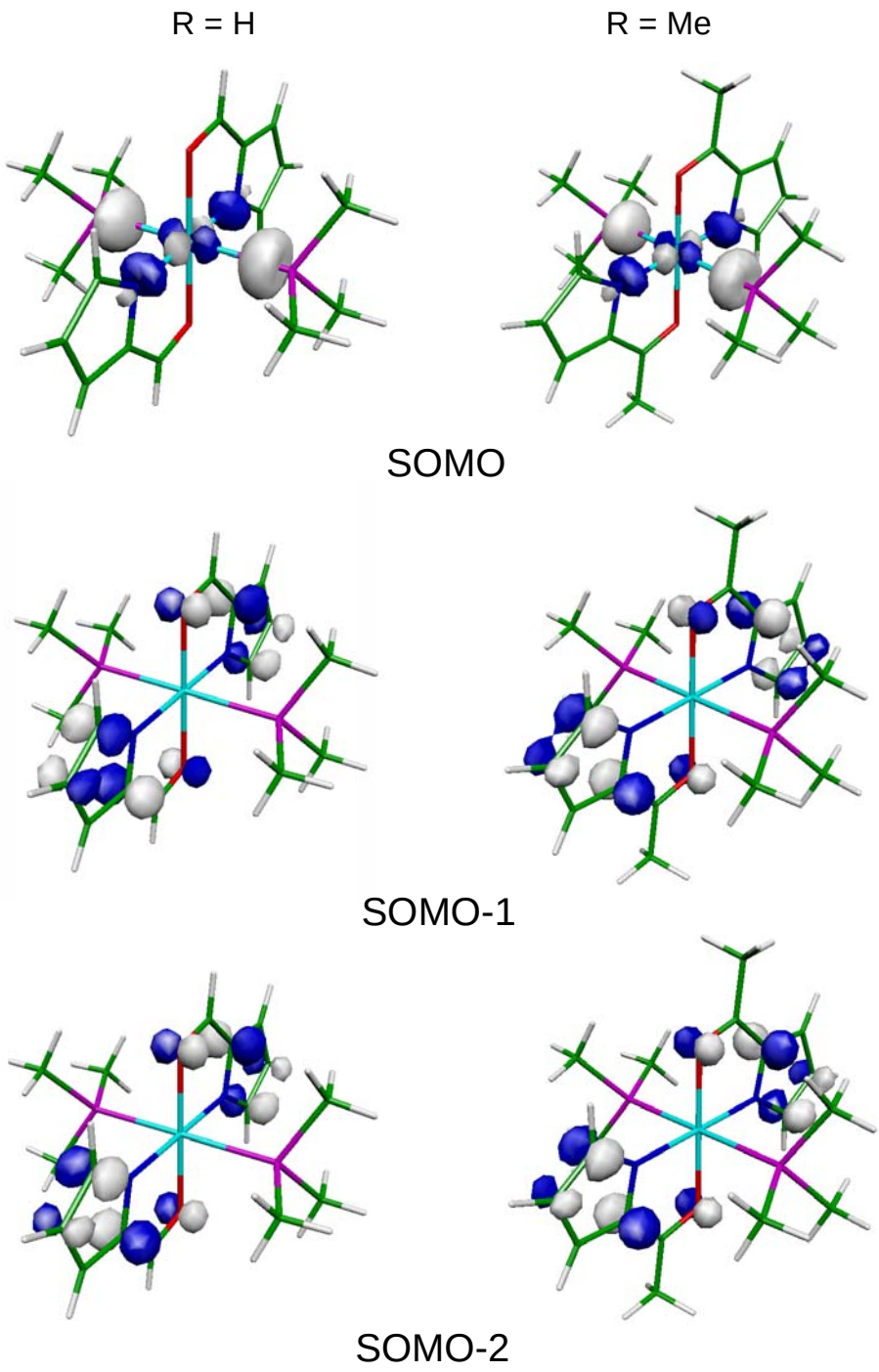

Fig. S3. Frontier orbitals (half filled) of the *S*=3/2 isomers of complexes **2a** (left) and **2b** (right).

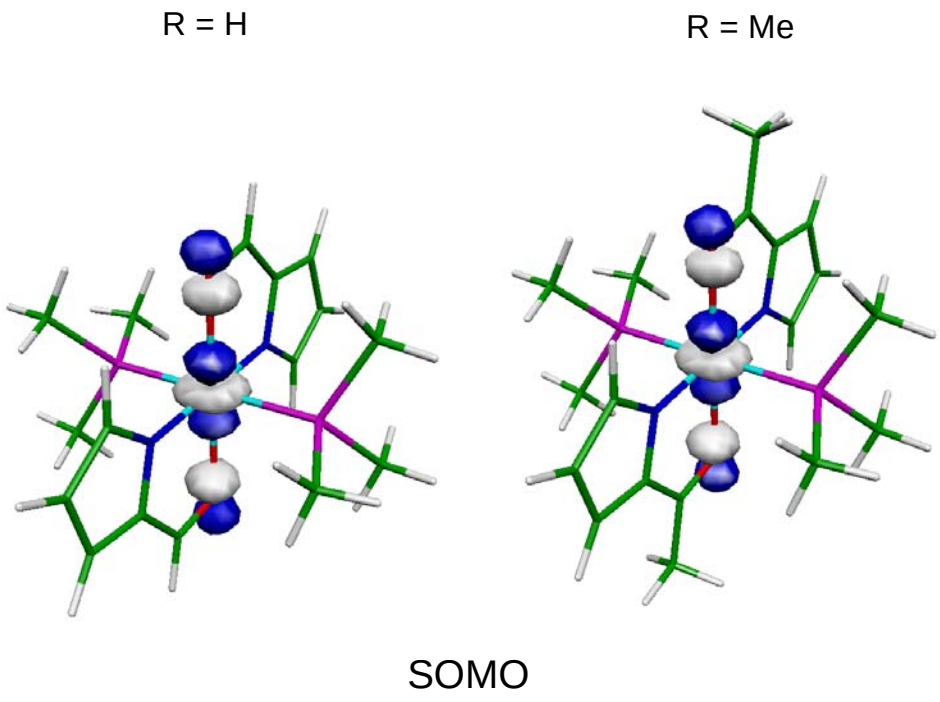

Fig. S4. Frontier orbitals (half filled) of the *S*=1/2 isomers of complexes **2a** (left) and **2b** (right).

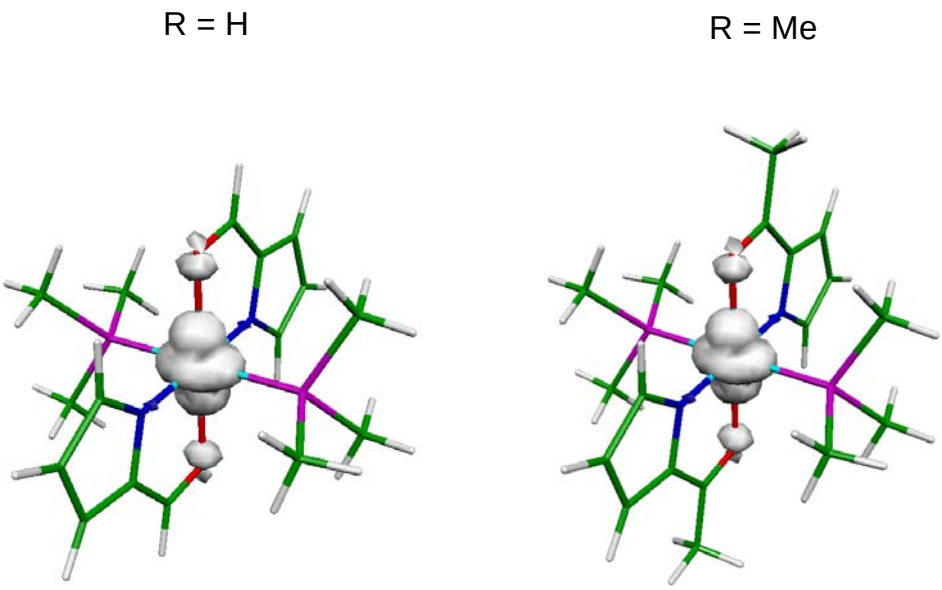

Fig. S5. Calculated spin density of the *S*=1/2 isomers of complexes **2a** (left) and **2b** (right).

Atomic Coordinates for the optimised [Co(N-N)$_2$] complexes (B3LYP/B1)

Isomer I, R = H, *S* = 1/2

Co	0.000059	-0.003166	-0.000643
N	-0.329707	-1.583593	-1.077190
P	-1.583990	-0.729534	1.646259
O	1.547487	-1.509035	0.925419
C	-1.173432	-1.922436	-2.083875
C	-0.963854	-3.285119	-2.467771
C	0.061350	-3.789185	-1.644059
C	0.446139	-2.718302	-0.781057
C	1.397726	-2.606209	0.268620
H	2.016504	-3.479386	0.523136
C	-0.877368	-0.860279	3.389367
C	-3.091712	0.374236	1.907557
C	-2.378140	-2.422731	1.404483
H	-1.880147	-1.208475	-2.486687
H	-1.499626	-3.815105	-3.244181
H	0.480519	-4.787343	-1.652505
N	0.329804	1.577325	1.075881
P	1.584357	0.723034	-1.647415
O	-1.547433	1.502853	-0.926938
C	1.173446	1.916230	2.082615
C	0.963885	3.278942	2.466397
C	-0.061395	3.782902	1.642723
C	-0.446087	2.712018	0.779678
C	-1.397662	2.599957	-0.270036
H	-2.016413	3.473159	-0.524542
C	0.877896	0.853651	-3.390602
H	-1.626044	-1.246810	4.091424
C	3.092132	-0.380716	-1.908504
H	-0.547838	0.130663	3.716058
C	2.378455	2.416265	-1.405688
H	-0.007485	-1.523504	3.370713
H	1.880155	1.202311	2.485512
H	-3.739206	-0.030452	2.694594
H	1.499618	3.808969	3.242807
H	-3.652684	0.445989	0.970889
H	-0.480631	4.781029	1.651168
H	-2.758920	1.377418	2.190111
H	-3.086604	-2.641369	2.212514
H	-1.599608	-3.191008	1.383885
H	-2.899282	-2.444779	0.442819
H	1.626638	1.240098	-4.092633
H	0.008028	1.516901	-3.372085
H	0.548363	-0.137310	-3.717230
H	3.739721	0.023989	-2.695458
H	2.759398	-1.383904	-2.191105
H	3.652975	-0.452467	-0.971761
H	3.086958	2.634873	-2.213693
H	2.899549	2.438377	-0.443999
H	1.599909	3.184529	-1.385170

Isomer II, R = H, *S* = 1/2

Co	0.136090	0.032393	0.121516
N	1.199338	-1.540498	0.509029
P	-1.544901	-0.732686	1.660075
O	-0.675089	-1.569144	-1.522422
C	2.184012	-1.831534	1.397434
C	2.606890	-3.187769	1.244424
C	1.832694	-3.740016	0.204412
C	0.962171	-2.702359	-0.243722
C	-0.016466	-2.642803	-1.275808
H	-0.202621	-3.547886	-1.874798
C	-0.898057	-1.174303	3.373836
C	-2.926948	0.488960	2.057210
C	-2.519072	-2.276493	1.183940
H	2.548309	-1.091222	2.096661
H	3.376811	-3.681990	1.822060
H	1.881515	-4.747881	-0.187882
N	0.851128	1.540451	1.598188
P	1.617652	0.718562	-1.637399
O	-1.013843	1.561504	-0.397828
C	1.678126	1.851768	2.620150
C	1.489850	3.212467	3.055568
C	0.485766	3.756153	2.244579
C	0.095729	2.709084	1.342344
C	-0.843803	2.649593	0.298930
H	-1.458737	3.518537	0.043665
C	0.699063	1.040000	-3.250299
H	-1.713209	-1.491349	4.035195
C	2.983959	-0.470372	-2.160797
H	-0.399529	-0.298441	3.800513
C	2.575868	2.322178	-1.371980
H	-0.165241	-1.981892	3.284351
H	2.379277	1.131736	3.025286
H	-3.630791	0.061169	2.781051
H	2.028197	3.705443	3.854734
H	-3.458089	0.740747	1.134224
H	0.079544	4.759131	2.280502
H	-2.493377	1.404568	2.471186
H	-3.285781	-2.503015	1.934694
H	-1.833016	-3.124964	1.100107
H	-2.989541	-2.114545	0.209790
H	1.382497	1.353546	-4.048912
H	-0.053349	1.815003	-3.076395
H	0.176452	0.123439	-3.538774
H	3.595939	-0.037489	-2.961276
H	2.537102	-1.405399	-2.510612
H	3.616646	-0.698801	-1.297545
H	3.165831	2.578864	-2.260201
H	3.241557	2.207258	-0.510927
H	1.876446	3.134197	-1.151880

Isomer III, R = H, *S* = 1/2

Co	0.627046	0.289129	0.225373
N	0.249765	-1.154592	-1.029156
P	1.242625	1.814098	1.920340
O	2.193286	-0.865630	0.709807
C	-0.668180	-1.527864	-1.945131
C	-0.390336	-2.858273	-2.412534
C	0.751295	-3.306277	-1.728010
C	1.142379	-2.234348	-0.864608
C	2.148413	-2.013309	0.091761
H	2.901690	-2.767146	0.336491
C	3.050067	1.717474	2.446738
C	0.993142	3.655205	1.596283
C	0.332850	1.579224	3.553558
H	-1.480716	-0.872929	-2.230912
H	-0.966665	-3.402805	-3.148706
H	1.239198	-4.267639	-1.822556
N	-1.053160	1.217490	-0.106050
P	2.210213	1.446069	-1.790050
O	-0.774058	-0.824965	1.741659
C	-1.510940	2.213529	-0.909785
C	-2.921941	2.369421	-0.757085
C	-3.335198	1.409252	0.189486
C	-2.162205	0.703242	0.584939
C	-1.945455	-0.361140	1.509412
H	-2.814141	-0.784062	2.036127
C	1.385615	1.377793	-3.499197
H	3.238685	2.333292	3.334123
C	3.730490	0.357593	-2.118759
H	3.691866	2.058118	1.627222
C	3.022857	3.167802	-1.892173
H	3.290689	0.671326	2.653504
H	-0.845969	2.772166	-1.555633
H	1.254663	4.248826	2.480317
H	-3.542425	3.087830	-1.276476
H	-0.055058	3.830957	1.335595
H	-4.339938	1.234168	0.552670
H	1.617982	3.970151	0.754706
H	0.735840	2.245665	4.325630
H	0.429571	0.536389	3.866740
H	-0.730115	1.793258	3.405375
H	2.110356	1.575266	-4.298900
H	0.580198	2.118267	-3.554134
H	0.948279	0.384643	-3.640832
H	4.295087	0.717072	-2.988117
H	3.398890	-0.669072	-2.302960
H	4.378157	0.355596	-1.236084
H	3.589288	3.284951	-2.824591
H	3.705805	3.304587	-1.045679
H	2.251412	3.944900	-1.846036

Isomer IV, R = H, *S* = 1/2

Co	0.385571	-0.127571	-0.074439
N	1.990282	-1.063533	0.509316
P	0.380522	1.872766	1.759495
O	0.222733	-2.022981	-1.350409
C	3.003798	-0.880524	1.396538
C	3.784428	-2.069002	1.516693

C	3.203399	-3.024188	0.658193
C	2.091569	-2.384451	0.040236
C	1.131117	-2.818485	-0.914260
H	1.176429	-3.851081	-1.288924
C	1.791221	2.364591	2.939249
C	-0.102463	3.582373	1.086026
C	-1.011316	1.604996	3.016903
H	3.140332	0.055971	1.918792
H	4.649121	-2.199794	2.153833
H	3.526631	-4.044296	0.494351
N	-1.391997	0.480081	-0.629380
P	1.742941	0.940621	-1.761278
O	-0.702229	-1.243675	1.269309
C	-2.012913	1.297134	-1.517146
C	-3.431989	1.129587	-1.453133
C	-3.683630	0.151825	-0.473961
C	-2.409823	-0.241433	0.030482
C	-1.967242	-1.146376	1.019571
H	-2.671299	-1.760372	1.590938
C	1.062523	2.138933	-3.060073
H	1.504150	3.220072	3.563362
C	2.636330	-0.302996	-2.861952
H	2.687786	2.626922	2.366518
C	3.184809	1.945512	-1.068925
H	2.028796	1.516165	3.590197
H	-1.463806	1.962445	-2.166500
H	-0.333379	4.280953	1.899703
H	-4.160034	1.657681	-2.054522
H	-0.982400	3.473942	0.443444
H	-4.644935	-0.234478	-0.161022
H	0.719418	3.995323	0.489214
H	-1.067889	2.437770	3.728837
H	-0.831139	0.670236	3.556401
H	-1.963413	1.518511	2.484181
H	1.870785	2.483211	-3.716400
H	0.606686	3.007420	-2.573423
H	0.305149	1.631304	-3.665523
H	3.290803	0.207788	-3.578498
H	1.893554	-0.899884	-3.398844
H	3.229861	-0.974001	-2.234859
H	3.848042	2.288416	-1.871955
H	3.750632	1.317563	-0.374920
H	2.801779	2.816310	-0.525836

Isomer V, R = H, *S* = 1/2

Co	0.630438	0.413799	-0.077280
N	0.445824	-1.115305	-1.286084
P	1.071478	1.954568	1.678398
O	2.121171	-1.075029	0.908063
C	-0.315034	-1.458589	-2.352791
C	-0.096218	-2.829640	-2.700778
C	0.840715	-3.337602	-1.782302
C	1.166504	-2.260487	-0.902217
C	2.008569	-2.168970	0.234712
H	2.577413	-3.056639	0.547524
C	2.826529	1.837912	2.365478
C	0.827930	3.808088	1.401989
C	0.051908	1.686789	3.241559
H	-0.987189	-0.749254	-2.817496
H	-0.575693	-3.362545	-3.511175
H	1.236880	-4.344063	-1.734978
N	-0.953029	-0.199330	0.883419
P	2.242429	1.250921	-1.625248
O	-0.982688	1.800703	-1.018038
C	-1.260919	-1.157831	1.786400
C	-2.669559	-1.163613	2.045789
C	-3.234577	-0.155155	1.244713
C	-2.152870	0.436152	0.520453
C	-2.095903	1.453723	-0.464741
H	-3.027109	1.955488	-0.765953
C	1.431113	1.528056	-3.303359
H	2.917969	2.381735	3.313084
C	3.662291	0.078981	-2.034607
H	3.544782	2.248116	1.648427
C	3.166679	2.891493	-1.419506
H	3.054818	0.778490	2.513568
H	-0.499768	-1.799062	2.211038
H	0.960645	4.363614	2.338013
H	-3.186791	-1.829422	2.723960
H	-0.182289	3.975619	1.016376
H	-4.279114	0.120323	1.172551
H	1.543733	4.177098	0.662423
H	0.338065	2.412593	4.012436
H	0.219115	0.672264	3.612364
H	-1.011799	1.791037	3.010439
H	2.132976	1.992316	-4.006321
H	0.554133	2.166393	-3.163111
H	1.099653	0.565707	-3.701955
H	4.284951	0.487033	-2.839594
H	3.247940	-0.884256	-2.344668
H	4.274145	-0.079216	-1.140854
H	3.855241	3.041399	-2.259515
H	3.740102	2.898452	-0.487728
H	2.447112	3.716049	-1.404577

Isomer I, R = Me, *S* = 1/2

Co	-0.000007	-0.000005	0.000000
N	-0.323630	-1.581913	-1.070565
P	-1.587450	-0.726816	1.649364
O	1.521565	-1.489101	0.910340
C	-1.172748	-1.908694	-2.077666
C	-0.971805	-3.267971	-2.469717
C	0.053162	-3.782047	-1.649941
C	0.448129	-2.720494	-0.780504
C	1.408121	-2.608992	0.276387
C	2.300386	-3.772459	0.662259
C	-0.885155	-0.850968	3.395370
C	-3.099656	0.372570	1.908187
C	-2.377814	-2.423439	1.414276
H	-1.875725	-1.186825	-2.472708
H	-1.511188	-3.792194	-3.247652
H	0.461590	-4.783977	-1.671651
H	2.034928	-4.693640	0.136272
H	2.237428	-3.940509	1.744436
H	3.345197	-3.522583	0.434649
N	0.323622	1.581905	1.070563
P	1.587438	0.726798	-1.649365
O	-1.521608	1.489145	-0.910352
C	1.172745	1.908678	2.077664
C	0.971763	3.267932	2.469771
C	-0.053112	3.782056	1.649912
C	-0.448124	2.720498	0.780502
C	-1.408123	2.609026	-0.276389
C	-2.300340	3.772527	-0.662265
C	0.885143	0.850943	-3.395372
H	-1.633547	-1.237618	4.097798
C	3.099644	-0.372589	-1.908183
H	-0.557916	0.141723	3.719109
C	2.377799	2.423424	-1.414283
H	-0.013244	-1.511679	3.379238
H	1.875709	1.186799	2.472711
H	-3.746468	-0.030288	2.696851
H	1.511112	3.792130	3.247745
H	-3.660591	0.437514	0.970867
H	-0.461506	4.784002	1.671602
H	-2.768712	1.377593	2.186992
H	-2.034846	4.693698	-0.136276
H	-3.086863	-2.642030	2.221941
H	-2.237370	3.940576	-1.744441
H	-1.596463	-3.189042	1.396633
H	-3.345162	3.522693	-0.434659
H	-2.896442	-2.450797	0.451332
H	1.633533	1.237600	-4.097799
H	0.013225	1.511644	-3.379244
H	0.557916	-0.141752	-3.719110
H	3.746459	0.030268	-2.696846
H	2.768701	-1.377612	-2.186987
H	3.660576	-0.437532	-0.970861
H	3.086847	2.642014	-2.221951
H	2.896429	2.450785	-0.451341
H	1.596447	3.189025	-1.396642

Isomer II, R = Me, *S* = 1/2

Co	-0.139652	0.068880	-0.166751
N	0.920076	-1.504786	0.216699
P	-1.819664	-0.699990	1.387710
O	-0.937171	-1.487322	-1.766506
C	1.907154	-1.791005	1.104802
C	2.330902	-3.145164	0.954793
C	1.554120	-3.701068	-0.082445
C	0.680099	-2.667998	-0.534063
C	-0.314080	-2.597212	-1.565189
C	-0.652059	-3.805940	-2.417404
C	-1.166309	-1.118972	3.105543
C	-3.213970	0.510962	1.780246
C	-2.783778	-2.258586	0.934851
H	2.271475	-1.047841	1.800816
H	3.102700	-3.638269	1.531013

H	1.610155	-4.711564	-0.465509
H	0.008819	-4.654475	-2.220375
H	-0.590649	-3.535779	-3.478789
H	-1.688862	-4.110253	-2.221905
N	0.550651	1.572032	1.291947
P	1.362562	0.763646	-1.917947
O	-1.286625	1.593469	-0.685234
C	1.383102	1.862998	2.317187
C	1.206291	3.217266	2.767113
C	0.204447	3.777719	1.961949
C	-0.196736	2.746547	1.048074
C	-1.144131	2.699247	-0.003026
C	-2.016441	3.872674	-0.381597
C	0.457427	1.091577	-3.538369
H	-1.976954	-1.433611	3.773702
C	2.730095	-0.425545	-2.440994
H	-0.670976	-0.235434	3.520067
C	2.324653	2.364997	-1.647491
H	-0.428566	-1.922837	3.021989
H	2.078340	1.131685	2.711811
H	-3.905189	0.088185	2.519203
H	1.748366	3.698838	3.570781
H	-3.758462	0.739047	0.858664
H	-0.188507	4.784825	2.016388
H	-2.785809	1.438087	2.174175
H	-1.786328	4.762593	0.209817
H	-3.542223	-2.488040	1.693222
H	-1.886596	4.102792	-1.446615
H	-2.088416	-3.099943	0.853210
H	-3.072245	3.609615	-0.236485
H	-3.264516	-2.108353	-0.036415
H	1.147784	1.393535	-4.335637
H	-0.286754	1.876108	-3.371273
H	-0.075838	0.180390	-3.824585
H	3.345395	0.006841	-3.239358
H	2.282838	-1.360156	-2.791920
H	3.359521	-0.656329	-1.575922
H	2.912683	2.627397	-2.535455
H	2.992528	2.243953	-0.788864
H	1.626824	3.176062	-1.418449

Isomer III, R = Me, *S* = 1/2

Co	0.452486	0.293090	0.330822
N	0.097629	-1.141023	-0.934857
P	1.068867	1.837753	2.008842
O	2.021623	-0.849428	0.800641
C	-0.817523	-1.505849	-1.859248
C	-0.533640	-2.827625	-2.339589
C	0.608668	-3.278353	-1.654156
C	0.992984	-2.216344	-0.778044
C	2.002056	-2.007244	0.192150
C	3.036179	-3.037711	0.565422
C	2.870814	1.740365	2.555841
C	0.836730	3.676558	1.658095
C	0.142161	1.633983	3.637092
H	-1.630014	-0.848611	-2.139787
H	-1.102553	-3.366602	-3.085684
H	1.098765	-4.237212	-1.762232
H	3.013290	-3.900262	-0.106510
H	2.848419	-3.384558	1.590302
H	4.036342	-2.587990	0.550219
N	-1.228973	1.212803	0.000401
P	2.051411	1.475517	-1.713121
O	-0.920992	-0.795029	1.820206
C	-1.677535	2.211422	-0.806358
C	-3.087160	2.370103	-0.663380
C	-3.508658	1.408583	0.279547
C	-2.342226	0.697132	0.683884
C	-2.119803	-0.381331	1.608345
C	-3.277409	-1.054101	2.319393
C	1.221121	1.396416	-3.419726
H	3.052578	2.362832	3.440108
C	3.558210	0.365742	-2.037494
H	3.521218	2.072893	1.739694
C	2.886560	3.185793	-1.843415
H	3.106618	0.695179	2.772899
H	-1.005756	2.767998	-1.446872
H	1.101222	4.281236	2.533768
H	-3.703822	3.090758	-1.184412
H	-0.209092	3.857311	1.391339
H	-4.518711	1.242505	0.630617
H	1.466743	3.972227	0.813304
H	-4.189964	-0.451545	2.292490
H	0.534763	2.315389	4.401515
H	-3.482692	-2.017801	1.833165
H	0.237668	0.597261	3.970745
H	-3.000931	-1.262878	3.358887
H	-0.919367	1.842948	3.471900
H	1.945194	1.577068	-4.224160
H	0.423277	2.144724	-3.480300
H	0.772805	0.406368	-3.548040
H	4.119656	0.705363	-2.916943
H	3.213040	-0.659737	-2.202704
H	4.213027	0.371789	-1.159972
H	3.454163	3.281817	-2.777662
H	3.571038	3.327555	-0.998840
H	2.124695	3.973054	-1.809127

Isomer IV, R = Me, *S* = 1/2

Co	0.607457	-0.140465	-0.133014
N	2.208893	-1.079163	0.446213
P	0.615466	1.879290	1.712635
O	0.457704	-2.011112	-1.392564
C	3.222270	-0.880390	1.331411
C	4.014739	-2.058430	1.453366
C	3.441152	-3.022366	0.597787
C	2.320611	-2.399240	-0.020589
C	1.348084	-2.842939	-0.975363
C	1.335073	-4.268287	-1.487508
C	2.022976	2.396138	2.887164
C	0.100191	3.582510	1.045653
C	-0.764989	1.588396	2.978158
H	3.348296	0.060140	1.849099
H	4.883406	-2.179415	2.087203
H	3.781935	-4.037302	0.439679
H	2.295805	-4.771074	-1.341385
H	1.068646	-4.276028	-2.550081
H	0.563547	-4.835740	-0.948716
N	-1.165665	0.479681	-0.673333
P	1.972408	0.936952	-1.811582
O	-0.486338	-1.238274	1.206258
C	-1.773631	1.309523	-1.560307
C	-3.192725	1.164448	-1.494678
C	-3.457194	0.187670	-0.515761
C	-2.190729	-0.227418	-0.013409
C	-1.759753	-1.154699	0.975087
C	-2.707115	-2.037841	1.748989
C	1.299996	2.122764	-3.126845
H	1.723561	3.244999	3.514684
C	2.887008	-0.306640	-2.895282
H	2.911287	2.676135	2.309794
C	3.401627	1.956223	-1.113505
H	2.280794	1.551024	3.534875
H	-1.213543	1.966711	-2.208353
H	-0.139018	4.275375	1.861935
H	-3.914845	1.705187	-2.092115
H	-0.780085	3.459914	0.406166
H	-4.426369	-0.179687	-0.204588
H	0.912561	4.010482	0.446249
H	-3.745943	-1.709220	1.652650
H	-0.838234	2.423850	3.685570
H	-2.630056	-3.066305	1.370977
H	-0.560242	0.661194	3.522087
H	-2.420120	-2.055554	2.806458
H	-1.716171	1.476535	2.448504
H	2.111247	2.457325	-3.784631
H	0.845394	2.998035	-2.651137
H	0.542187	1.610823	-3.728157
H	3.549461	0.203751	-3.604931
H	2.153707	-0.908088	-3.440204
H	3.473826	-0.972411	-2.256359
H	4.068888	2.299908	-1.912919
H	3.965813	1.335588	-0.411619
H	3.007348	2.826721	-0.578113

Isomer V, R = Me, *S* = 1/2

Co	-0.069509	-0.017703	-0.004123
N	-0.234172	-1.546530	-1.211266
P	0.360507	1.522102	1.758117
O	1.402640	-1.493239	0.965326
C	-0.990664	-1.873284	-2.287184
C	-0.772405	-3.237568	-2.651640
C	0.160053	-3.758053	-1.733976
C	0.484945	-2.695328	-0.836628
C	1.326439	-2.608988	0.314775
C	2.134118	-3.797582	0.797307
C	2.111277	1.406441	2.457298
C	0.120431	3.377351	1.486347

C	-0.668600	1.252823	3.315186
H	-1.658510	-1.155398	-2.744819
H	-1.247175	-3.761147	-3.470953
H	0.549973	-4.767152	-1.705763
H	2.006129	-4.675748	0.159078
H	1.831585	-4.053125	1.821113
H	3.197773	-3.528760	0.831738
N	-1.657340	-0.629583	0.943652
P	1.548260	0.826798	-1.544444
O	-1.673402	1.343508	-0.933293
C	-1.948947	-1.593713	1.847146
C	-3.353598	-1.615025	2.113363
C	-3.932666	-0.610216	1.315705
C	-2.863299	-0.004360	0.585631
C	-2.812039	1.019759	-0.408743
C	-4.066520	1.730077	-0.878474
C	0.741115	1.122213	-3.221832
H	2.194615	1.941659	3.410606
C	2.962733	-0.348341	-1.964518
H	2.832809	1.825923	1.748827
C	2.484200	2.460073	-1.326844
H	2.341827	0.346295	2.596605
H	-1.176936	-2.225126	2.266706
H	0.250864	3.931237	2.423744
H	-3.862380	-2.286048	2.792930
H	-0.888627	3.546220	1.098211
H	-4.981984	-0.352311	1.255222
H	0.838664	3.747019	0.749306
H	-4.942030	1.469479	-0.277660
H	-0.389858	1.979345	4.088219
H	-3.910101	2.815340	-0.843823
H	-0.501695	0.238461	3.686633
H	-4.265025	1.463630	-1.925284
H	-1.731006	1.353074	3.076266
H	1.445337	1.590193	-3.920050
H	-0.134096	1.761799	-3.076379
H	0.406491	0.164367	-3.628622
H	3.588673	0.063658	-2.765037
H	2.543022	-1.306365	-2.283506
H	3.572520	-0.516571	-1.071071
H	3.172441	2.613551	-2.166552
H	3.058935	2.454229	-0.395737
H	1.770310	3.289439	-1.302439

Isomer I, R = H, *S* = 3/2

Co	-0.006138	0.000599	-0.011669
P	1.653305	-1.703691	-1.208705
N	1.546647	0.930758	0.987549
O	0.595093	1.505641	-1.497023
C	2.215994	0.878591	2.165316
C	3.243145	1.877654	2.207655
C	3.186526	2.571219	0.984641
C	2.127576	1.971152	0.235188
C	1.578457	2.216120	-1.046558
C	1.553741	-1.638410	-3.096169
C	3.512602	-1.519234	-0.908546
C	1.395814	-3.548899	-0.877574
H	1.959125	0.152310	2.926203
H	3.925867	2.053964	3.028660
H	3.814059	3.393977	0.665992
H	1.986918	3.018811	-1.674083
P	-1.666070	1.705271	1.185123
N	-1.559222	-0.929316	-1.010699
O	-0.607303	-1.504384	1.473749
C	-2.228940	-0.876933	-2.188246
C	-3.256528	-1.875558	-2.230199
C	-3.199567	-2.569318	-1.007313
C	-2.140208	-1.969574	-0.258176
H	2.253598	-2.342441	-3.563087
C	-1.590873	-2.214675	1.023457
H	1.777688	-0.619886	-3.428547
C	-1.408509	3.550488	0.853995
H	0.531499	-1.881048	-3.403876
C	-1.567876	1.640309	3.072666
H	4.088924	-2.242302	-1.498875
C	-3.525128	1.520648	0.883517
H	3.721359	-1.668630	0.155828
H	-1.972130	-0.150692	-2.949191
H	3.822529	-0.503168	-1.173351
H	-3.939655	-2.051556	-3.050934
H	2.090813	-4.161608	-1.464725
H	-3.827179	-3.391958	-0.688518
H	0.366825	-3.818888	-1.136535
H	-1.999390	-3.017273	1.651062
H	1.547795	-3.747649	0.188445
H	-2.104205	4.163196	1.440324
H	-1.559391	3.749061	-0.212213
H	-0.379831	3.820664	1.114003
H	-2.267222	2.345287	3.538918
H	-0.545559	1.881788	3.381027
H	-1.793281	0.622146	3.405172
H	-4.102142	2.242325	1.474873
H	-3.834798	0.503918	1.146049
H	-3.733255	1.672094	-0.180698

Isomer II, R = H, *S* = 3/2

Co	0.264362	-0.283044	0.240669
N	1.613481	-1.458584	1.318481
P	1.778921	0.274763	-1.810190
O	0.086015	-2.212685	-0.810512
C	2.472817	-1.390023	2.365656
C	3.109016	-2.654009	2.588372
C	2.601717	-3.538064	1.619063
C	1.674761	-2.782263	0.836972
C	0.852941	-3.102383	-0.270029
H	0.862571	-4.119782	-0.682253
C	0.916157	-0.200063	-3.419371
C	2.245873	2.080757	-2.122149
C	3.454200	-0.586978	-1.982730
H	2.619027	-0.471998	2.920795
H	3.838738	-2.872806	3.356946
H	2.856730	-4.581481	1.483251
N	0.268343	1.586288	1.173855
P	-1.740795	-1.082145	1.796640
O	-1.218354	0.812138	-0.977272
C	0.848540	2.250315	2.204699
C	0.334678	3.583512	2.307906
C	-0.613119	3.731936	1.279207
C	-0.643326	2.484681	0.582815
C	-1.380726	2.014212	-0.529811
H	-2.102452	2.675604	-1.026683
C	-1.363776	-0.860038	3.636801
H	1.533522	0.029736	-4.296590
C	-2.267573	-2.898200	1.733902
H	-0.033248	0.340585	-3.473818
C	-3.405855	-0.197491	1.640887
H	0.689478	-1.269783	-3.387729
H	1.598227	1.782955	2.830674
H	2.776524	2.197625	-3.075115
H	0.628587	4.324290	3.039982
H	2.882119	2.439576	-1.306288
H	-1.204532	4.609754	1.051405
H	1.336034	2.689118	-2.136855
H	3.932101	-0.339433	-2.938549
H	3.311101	-1.670425	-1.918968
H	4.108421	-0.281087	-1.159637
H	-2.207396	-1.178327	4.261404
H	-1.144278	0.194998	3.830898
H	-0.477884	-1.450064	3.893612
H	-3.054829	-3.111470	2.467515
H	-1.398590	-3.531026	1.942162
H	-2.631799	-3.132068	0.728431
H	-4.134113	-0.585430	2.363662
H	-3.790303	-0.334122	0.625095
H	-3.260155	0.873931	1.814093

Isomer III, R = H, *S* = 3/2

Co	-0.304861	0.505699	-0.484705
N	-0.686460	-1.166863	-1.638575
O	0.955367	-1.008232	0.548867
C	-1.398474	-1.566577	-2.726088
C	-1.282601	-2.977057	-2.921867
C	-0.451647	-3.459812	-1.891494
C	-0.090169	-2.326307	-1.106304
C	0.744088	-2.168747	0.031595
H	1.225998	-3.049674	0.476075
H	-1.961489	-0.864049	-3.328234
H	-1.748805	-3.552148	-3.711171
H	-0.142680	-4.483492	-1.721748
N	-1.658648	0.310310	1.079047
P	-1.900348	2.234576	-1.694896
P	2.018696	1.096139	-1.596694
O	0.299176	2.178905	0.814296
C	-2.649470	-0.510026	1.500667
C	-3.087841	-0.140170	2.815308
C	-2.304808	0.959011	3.209173
C	-1.419362	1.228697	2.118936
C	-0.376207	2.160584	1.920001

H	-0.128245	2.884574	2.706414
C	-1.626923	2.877420	-3.458907
C	2.769501	-0.168568	-2.786515
C	3.332576	1.210685	-0.246806
C	-2.158208	3.853145	-0.751955
C	2.315281	2.714796	-2.537113
H	3.791638	0.107380	-3.073693
C	-3.679132	1.595767	-1.810978
H	2.146131	-0.241766	-3.684053
H	2.781831	-1.151087	-2.304307
H	-3.007996	-1.324778	0.883936
H	4.329093	1.394241	-0.667488
H	-3.866295	-0.628355	3.386966
H	3.327839	0.276905	0.322517
H	-2.350019	1.495753	4.148365
H	3.053954	2.021892	0.432260
H	3.375543	2.833218	-2.792527
H	2.003197	3.554780	-1.907487
H	1.725221	2.724155	-3.460227
H	-2.453249	3.525540	-3.775521
H	-1.548418	2.032890	-4.152272
H	-0.692618	3.447228	-3.498435
H	-2.877577	4.501578	-1.266806
H	-1.199693	4.370705	-0.649769
H	-2.530845	3.622415	0.250927
H	-4.358925	2.376214	-2.173968
H	-3.997959	1.264785	-0.817798
H	-3.721559	0.736425	-2.488151

Isomer IV, R = H, *S* = 3/2

Co	-0.027905	0.596192	0.008899
N	1.051351	0.746494	-1.768018
O	-1.116483	2.203694	-0.992977
C	2.106503	0.201963	-2.427006
C	2.377487	0.914306	-3.637299
C	1.428844	1.951656	-3.714071
C	0.614112	1.832603	-2.549004
C	-0.514815	2.549977	-2.080416
H	-0.893977	3.408176	-2.649620
H	2.637540	-0.659075	-2.039760
H	3.164414	0.691891	-4.346089
H	1.329679	2.695444	-4.494566
N	-1.112139	0.727696	1.782397
P	1.728418	-1.040663	1.180758
P	-1.730898	-1.100204	-1.158449
O	1.022348	2.234330	1.006256
C	-2.156644	0.162026	2.440633
C	-2.450054	0.875419	3.644975
C	-1.527187	1.935959	3.718845
C	-0.704806	1.829245	2.558002
C	0.407750	2.571734	2.089307
H	0.762915	3.442540	2.654886
C	2.181001	-2.781069	0.572482
C	-1.384226	-1.447305	-2.985112
C	-3.454325	-0.321887	-1.244609
C	1.405675	-1.371946	3.014689
C	-2.143859	-2.843917	-0.531486
H	-2.208770	-2.004447	-3.446731
C	3.430395	-0.214626	1.240936
H	-0.456779	-2.020938	-3.080456
H	-1.244666	-0.497106	-3.509304
H	-2.665471	-0.713833	2.056921
H	-4.137671	-0.928111	-1.852019
H	-3.234361	0.638528	4.351974
H	-3.361366	0.680751	-1.671707
H	-1.449523	2.687035	4.494789
H	-3.858110	-0.214683	-0.232815
H	-2.943373	-3.299116	-1.128902
H	-2.464884	-2.794529	0.514696
H	-1.251567	-3.477047	-0.591309
H	2.996813	-3.208590	1.168302
H	2.491698	-2.736548	-0.477046
H	1.305487	-3.435584	0.647909
H	2.248191	-1.900704	3.477215
H	0.494452	-1.968412	3.125377
H	1.245177	-0.418593	3.527027
H	4.134865	-0.791723	1.852469
H	3.312489	0.791889	1.652526
H	3.823351	-0.112593	0.224401

Isomer V, R = H, *S* = 3/2

Co	0.230949	0.113512	0.437646
N	0.327774	-1.828353	-0.346226
O	1.480154	-0.844550	1.925228
C	-0.050949	-2.567858	-1.413869
C	0.508048	-3.888038	-1.344326
C	1.275114	-3.940995	-0.168676
C	1.156494	-2.652488	0.443030
C	1.723669	-2.077017	1.600694
H	2.383841	-2.672407	2.243663
H	-0.682975	-2.156402	-2.190881
H	0.366162	-4.677852	-2.070409
H	1.850671	-4.778757	0.204283
N	1.619457	0.854539	-0.952701
P	0.667635	2.364498	1.796198
P	-1.970240	-0.672765	1.704448
O	-1.097768	1.133627	-0.929997
C	2.936565	0.838651	-1.261107
C	3.176888	1.507298	-2.508467
C	1.927781	1.942461	-2.981198
C	0.966090	1.528829	-2.005115
C	-0.439830	1.631210	-1.931856
H	-0.996510	2.137694	-2.730105
C	-0.133418	2.795948	3.460625
C	-1.853671	-2.192543	2.825331
C	-3.200856	-1.253231	0.391957
C	0.483486	4.000676	0.864450
C	-3.073884	0.468355	2.741809
H	-2.847654	-2.537298	3.136129
C	2.498105	2.394291	2.268292
H	-1.260986	-1.947404	3.713126
H	-1.344692	-2.994725	2.281748
H	3.662365	0.357030	-0.617809
H	-4.155455	-1.553026	0.841349
H	4.139414	1.635076	-2.986345
H	-2.769680	-2.101081	-0.149176
H	1.721672	2.476267	-3.900328
H	-3.359312	-0.435812	-0.317891
H	-3.987199	-0.051421	3.056607
H	-3.349321	1.343794	2.143849
H	-2.530707	0.805711	3.630513
H	0.313776	3.702105	3.887427
H	0.012629	1.963518	4.157466
H	-1.207599	2.957932	3.324629
H	0.881242	4.839772	1.448379
H	-0.574562	4.180447	0.645720
H	1.024497	3.929474	-0.084196
H	2.744997	3.284934	2.859060
H	3.099416	2.384523	1.354051
H	2.724075	1.488354	2.838568

Isomer I, R = Me, *S* = 3/2

Co	0.000018	0.000023	0.000012
N	-0.365569	-1.643939	-1.192099
P	-1.767027	-0.793932	1.841594
O	1.346656	-1.470090	0.876991
C	-1.138143	-2.008634	-2.245932
C	-0.886534	-3.370456	-2.606633
C	0.096079	-3.850244	-1.719127
C	0.410015	-2.766108	-0.842650
C	1.304949	-2.610251	0.256868
C	2.211990	-3.728044	0.722859
C	-1.004632	-0.954666	3.565410
C	-3.260055	0.314649	2.199835
C	-2.594007	-2.483709	1.630192
H	-1.832297	-1.313289	-2.700984
H	-1.366148	-3.917535	-3.407955
H	0.526490	-4.843218	-1.701772
H	2.045803	-4.654763	0.167120
H	2.051111	-3.912406	1.792413
H	3.259432	-3.422026	0.602638
N	0.365599	1.643985	1.192117
P	1.767059	0.793981	-1.841573
O	-1.346601	1.469898	-0.876844
C	1.138148	2.008715	2.245955
C	0.886645	3.370602	2.606491
C	-0.096203	3.850250	1.719165
C	-0.410018	2.766113	0.842648
C	-1.304919	2.610144	-0.256876
C	-2.212097	3.727815	-0.722897
C	1.004657	0.954724	-3.565385
H	-1.728845	-1.342501	4.292624
C	3.260087	-0.314596	-2.199828
H	-0.652726	0.029946	3.890032
C	2.594040	2.483757	-1.630166
H	-0.140705	-1.624277	3.508925
H	1.832337	1.313407	2.701010
H	-3.857147	-0.075054	3.033579

H	1.366347	3.917759	3.407707
H	-3.886925	0.378716	1.304055
H	-0.526701	4.843187	1.701833
H	-2.904518	1.320186	2.447891
H	-2.045989	4.654584	-0.167218
H	-3.252867	-2.718309	2.475553
H	-2.051276	3.912132	-1.792467
H	-1.821744	-3.255314	1.545880
H	-3.259503	3.421695	-0.602621
H	-3.174639	-2.487296	0.701964
H	1.728865	1.342568	-4.292601
H	0.140727	1.624331	-3.508891
H	0.652753	-0.029887	-3.890013
H	3.857174	0.075112	-3.033572
H	2.904550	-1.320132	-2.447888
H	3.886961	-0.378667	-1.304051
H	3.252896	2.718364	-2.475529
H	3.174675	2.487340	-0.701941
H	1.821776	3.255361	-1.545846

Isomer II, R = Me, *S* = 3/2

Co	0.049862	0.014594	-0.052314
N	1.387584	-1.170078	1.022900
P	1.613963	0.603579	-2.071170
O	-0.109584	-1.888748	-1.100704
C	2.234346	-1.096229	2.080989
C	2.869485	-2.356520	2.312960
C	2.374187	-3.243062	1.338131
C	1.454403	-2.493129	0.542582
C	0.637710	-2.813740	-0.581557
C	0.612436	-4.198743	-1.190745
C	0.774536	0.158178	-3.702112
C	2.100197	2.410220	-2.353936
C	3.286438	-0.266590	-2.236384
H	2.370802	-0.176080	2.635061
H	3.590921	-2.574505	3.089649
H	2.638115	-4.285319	1.213805
H	1.291039	-4.888075	-0.681453
H	0.888396	-4.139446	-2.251328
H	-0.408407	-4.599244	-1.146319
N	0.036011	1.884326	0.870514
P	-1.932662	-0.779791	1.552711
O	-1.417716	1.092190	-1.256633
C	0.619245	2.544672	1.903110
C	0.103467	3.874132	2.012827
C	-0.849060	4.022917	0.987000
C	-0.880503	2.779694	0.284092
C	-1.623787	2.301669	-0.835078
C	-2.651487	3.155838	-1.545221
C	-1.516799	-0.542431	3.382713
H	1.411743	0.384069	-4.566196
C	-2.458414	-2.598072	1.520495
H	-0.164778	0.714839	-3.770267
C	-3.604835	0.098916	1.430590
H	0.528092	-0.907569	-3.683082
H	1.372351	2.075298	2.523435
H	2.623193	2.540385	-3.309554
H	0.397190	4.614537	2.745470
H	2.749094	2.744713	-1.537573
H	-1.439159	4.904169	0.771112
H	1.198085	3.030249	-2.345147
H	-2.695480	4.171722	-1.143784
H	3.783814	-0.000857	-3.177413
H	-2.418417	3.198904	-2.616500
H	3.134269	-1.350155	-2.199740
H	-3.641083	2.690199	-1.450026
H	3.927560	0.014248	-1.394283
H	-2.346602	-0.855164	4.028455
H	-1.292903	0.514266	3.561932
H	-0.625141	-1.130141	3.624327
H	-3.216096	-2.810790	2.284860
H	-1.578961	-3.225817	1.698781
H	-2.861622	-2.837945	0.531198
H	-4.311168	-0.274849	2.182154
H	-4.019947	-0.059304	0.429864
H	-3.454624	1.173570	1.578802

Isomer III, R = Me, *S* = 3/2

Co	-0.213804	0.190282	-0.356435
N	-0.575773	-1.480613	-1.508870
O	1.041176	-1.305529	0.654257
C	-1.283015	-1.866739	-2.605330
C	-1.169988	-3.273475	-2.812703
C	-0.346529	-3.767184	-1.779866
C	0.015024	-2.643866	-0.980818
C	0.846643	-2.489376	0.173402
C	1.493186	-3.674054	0.857945
H	-1.839646	-1.155491	-3.203128
H	-1.631315	-3.841907	-3.609781
H	-0.045426	-4.795161	-1.625084
H	1.429952	-4.586017	0.258026
H	0.989928	-3.848709	1.818489
H	2.543334	-3.448197	1.077061
N	-1.565177	-0.001186	1.206466
P	-1.843589	1.908143	-1.562194
P	2.087744	0.802054	-1.527778
O	0.377357	1.840592	0.934921
C	-2.560592	-0.824512	1.614415
C	-3.001583	-0.468092	2.929475
C	-2.215207	0.625434	3.336950
C	-1.324446	0.905853	2.254390
C	-0.267966	1.840713	2.063584
C	0.141187	2.827048	3.134525
C	-1.595635	2.599221	-3.312586
C	2.821269	-0.462838	-2.728914
C	3.428649	0.917449	-0.203260
C	-2.128539	3.501214	-0.582918
C	2.373754	2.419732	-2.474891
H	3.840030	-0.188785	-3.029973
C	-3.612547	1.242055	-1.683014
H	2.185440	-0.534634	-3.617758
H	2.836863	-1.445742	-2.247549
H	-2.918621	-1.630289	0.985640
H	4.417899	1.097791	-0.642361
H	-3.784621	-0.957337	3.494135
H	3.432460	-0.014878	0.368619
H	-2.269679	1.149368	4.282573
H	3.164767	1.730994	0.479001
H	-0.559810	2.841115	3.973443
H	3.429630	2.534892	-2.749560
H	1.136257	2.556038	3.512187
H	2.075229	3.261474	-1.840871
H	0.217892	3.832842	2.703907
H	1.766755	2.430115	-3.386955
H	-2.435905	3.239872	-3.607286
H	-1.507529	1.773539	-4.027234
H	-0.671817	3.186500	-3.344962
H	-2.869556	4.142934	-1.075193
H	-1.181140	4.039469	-0.482804
H	-2.482572	3.239964	0.419178
H	-4.306168	2.016142	-2.033498
H	-3.922328	0.892885	-0.693178
H	-3.642997	0.390988	-2.371236

Isomer IV, R = Me, *S* = 3/2

Co	0.082246	0.010288	0.030188
N	1.145209	0.152638	-1.746753
O	-0.994068	1.602620	-0.980393
C	2.195746	-0.415305	-2.395426
C	2.475952	0.275586	-3.612973
C	1.538456	1.323785	-3.704305
C	0.719691	1.232934	-2.540173
C	-0.407518	1.975590	-2.072068
C	-0.929408	3.192048	-2.803692
H	2.714805	-1.276859	-1.993514
H	3.259604	0.034965	-4.319575
H	1.454607	2.052607	-4.500145
H	-0.502039	3.288020	-3.805566
H	-0.675459	4.091196	-2.226217
H	-2.022638	3.145650	-2.869888
N	-0.987176	0.132633	1.803462
P	1.843096	-1.638957	1.204594
P	-1.624990	-1.699526	-1.140544
O	1.117306	1.633738	1.036483
C	-2.025759	-0.457727	2.451395
C	-2.329445	0.234099	3.662734
C	-1.419765	1.306756	3.750921
C	-0.593483	1.229094	2.591187
C	0.515956	1.998036	2.123145
C	1.001903	3.232713	2.849000
C	2.298711	-3.387416	0.620062
C	-1.276980	-2.028648	-2.970678
C	-3.347185	-0.917040	-1.223559
C	1.519111	-1.949372	3.042283
C	-2.045902	-3.450002	-0.536102
H	-2.102200	-2.578778	-3.439716
C	3.545816	-0.812985	1.259449
H	-0.350558	-2.603204	-3.070290

H	-1.132745	-1.073348	-3.484223
H	-2.521041	-1.334865	2.053286
H	-4.028831	-1.511022	-1.844983
H	-3.109857	-0.021891	4.367517
H	-3.247911	0.092381	-1.633024
H	-1.358400	2.043137	4.541865
H	-3.756430	-0.825571	-0.212330
H	0.572343	3.320509	3.850727
H	-2.846333	-3.895222	-1.139927
H	2.096021	3.219152	2.914593
H	-2.367667	-3.412621	0.510388
H	0.720756	4.121322	2.267775
H	-1.155514	-4.085222	-0.602833
H	3.113385	-3.807333	1.222967
H	2.611293	-3.356541	-0.429448
H	1.422916	-4.040914	0.702030
H	2.360829	-2.473338	3.511939
H	0.607061	-2.543462	3.158620
H	1.357400	-0.990111	3.543085
H	4.247689	-1.379128	1.884217
H	3.424231	0.200230	1.653300
H	3.943766	-0.727817	0.243234

Isomer V, R = Me, *S* = 3/2

Co	0.360299	0.125949	0.316507
N	0.413315	-1.833965	-0.404762
O	1.638449	-0.804699	1.770199
C	-0.022694	-2.588763	-1.440785
C	0.509871	-3.916364	-1.361046
C	1.320441	-3.957513	-0.212826
C	1.253950	-2.654428	0.373810
C	1.878286	-2.056070	1.503246
C	2.819359	-2.820565	2.407250
H	-0.674876	-2.180072	-2.202497
H	0.325485	-4.720840	-2.061124
H	1.889272	-4.803079	0.151772
H	2.886654	-3.877239	2.135563
H	2.481680	-2.733675	3.447578
H	3.821165	-2.374567	2.352845
N	1.679325	0.841348	-1.138584
P	0.842716	2.396081	1.641794
P	-1.825444	-0.621640	1.671658
O	-1.000115	1.143227	-1.001190
C	2.987053	0.801467	-1.486378
C	3.200632	1.469747	-2.735661
C	1.943882	1.929449	-3.167212
C	1.003675	1.530812	-2.165076
C	-0.408288	1.650906	-2.043754
C	-1.253773	2.346526	-3.087111
C	0.210892	2.767192	3.391540
C	-1.701376	-2.155804	2.773538
C	-3.106656	-1.173895	0.395042
C	0.471505	4.029296	0.760571
C	-2.884340	0.519464	2.757310
H	-2.692255	-2.494117	3.101271
C	2.709660	2.523937	1.914448
H	-1.089023	-1.925961	3.652240
H	-1.211907	-2.956363	2.210003
H	3.721881	0.303999	-0.865867
H	-4.050819	-1.464444	0.871873
H	4.149096	1.583000	-3.244489
H	-2.703744	-2.023274	-0.165079
H	1.727485	2.470255	-4.079477
H	-3.274824	-0.348770	-0.303475
H	-0.648654	2.783000	-3.885969
H	-3.795929	0.007864	3.090383
H	-1.958026	1.627397	-3.525487
H	-3.164292	1.408043	2.181032
H	-1.849912	3.135384	-2.611265
H	-2.311369	0.835092	3.635503
H	0.674409	3.677288	3.791943
H	0.454892	1.923112	4.045629
H	-0.876072	2.897916	3.375721
H	0.875546	4.886050	1.313797
H	-0.612144	4.146393	0.651837
H	0.918043	3.999334	-0.238441
H	2.974412	3.441357	2.454535
H	3.211314	2.513144	0.942172
H	3.037788	1.647580	2.481946