

Supporting Information

**DFT study of intramolecular interring η^6,η^6 -haptotropic
rearrangements in tricarbonylchromium complexes of 2-aminobiphenyl
and 4-aminobiphenyl**

Curtis J. Czerwinski, Evgenii O. Fetisov, Igor P. Gloriozov and Yuri F. Oprunenko

Section S1. Cartesian coordinates of stationary points discussed in the paper and their total energies (geometries were optimized in gas phase by PBE/TZV2p; energies are given in a.u., coordinates are given in Å)

1 → 2

1

E = -236.382971 E0 = -236.163321
24 -1.35883195 -0.17591830 1.68177891
6 -0.27683117 1.31305076 1.61361213
6 -0.89688481 -0.62403188 -0.49915602
6 -2.08341867 0.18015692 -0.38936713
6 -3.17261995 -0.22713303 0.41040793
6 -3.10448076 -1.44354731 1.15204238
6 -1.93387168 -2.22798516 1.08314004
6 -0.83979179 -1.82120726 0.26403088
6 0.22345922 -0.21209450 -1.37528959
6 1.56737462 -0.45352614 -1.02647600
6 2.61118682 -0.08151586 -1.86797534
6 2.35289890 0.55270512 -3.10267142
6 1.01015812 0.79545738 -3.45792712
6 -0.02862226 0.42360685 -2.60631405
6 -2.29731757 0.64818000 3.03199048
8 -2.89945592 1.16586887 3.88861141
8 0.48558938 -1.28692666 3.78402606
6 -0.23221669 -0.85155868 2.97178780
1 -2.12148279 1.14395591 -0.89494923
1 -4.04465146 0.41874644 0.50366270
1 -3.92412169 -1.73497061 1.80662571
1 -1.84822954 -3.13300088 1.68299089
1 0.05815771 -2.43655594 0.22785720
1 1.80141928 -0.89940981 -0.05788759

1	3.64372726	-0.26491277	-1.56207099
7	3.39380690	0.87785466	-3.96941668
1	0.78201555	1.27434364	-4.41280007
1	-1.05747431	0.60913727	-2.92110925
8	0.41262518	2.25358698	1.56454096
1	3.19292479	1.60941970	-4.64403766
1	4.30690572	0.98479227	-3.53870567

1-TS1

E = -236.332205 E0 = -236.114253

24	-0.70143458	0.19563001	1.30208271
6	-0.22775813	1.94004927	1.19733982
6	-1.16460018	-0.87127946	-0.57551200
6	-2.36017117	-0.09638606	-0.54863404
6	-3.46256306	-0.49092846	0.23561876
6	-3.38982232	-1.61604511	1.06331374
6	-2.17146621	-2.31088238	1.14816324
6	-1.08134240	-1.97973461	0.32114517
6	0.02598932	-0.41844365	-1.33098832
6	1.33126350	-0.84259353	-0.98012342
6	2.45456665	-0.38066698	-1.65845473
6	2.32712255	0.52418013	-2.73213219
6	1.02539909	0.93217261	-3.11033908
6	-0.08867627	0.47849265	-2.42110067
6	-1.64317153	0.57248368	2.79931200
8	-2.25056553	0.81872550	3.77265994
8	1.70228162	-0.20245426	3.02818738
6	0.75598234	-0.04968026	2.34879236
1	-2.43766987	0.80417570	-1.15544752
1	-4.37099855	0.11307889	0.21082533
1	-4.23289443	-1.89994293	1.69203646

1	-2.06965058	-3.14996081	1.83824318
1	-0.19508134	-2.61164357	0.33378152
1	1.48341714	-1.52043598	-0.14106782
1	3.44655790	-0.70832429	-1.34137369
7	3.43620296	0.95949832	-3.43633491
1	0.89901688	1.61505092	-3.95314998
1	-1.07251798	0.81157206	-2.75302680
8	0.09009824	3.06855420	1.13150710
1	3.33089078	1.81292577	-3.97447767
1	4.33354157	0.87938062	-2.96989425

1-IM

E = -236.338762 E0 = -236.120485

24	-0.18291518	0.83611977	0.57614841
6	-1.11622334	2.06141513	1.54976244
6	-1.23404929	-0.86336565	-0.49711916
6	-2.25402880	0.13217679	-0.39821870
6	-3.44998379	-0.13877063	0.30752201
6	-3.62545020	-1.35841005	0.94492598
6	-2.61079432	-2.33909282	0.88074337
6	-1.43506140	-2.09599125	0.18577376
6	0.03223800	-0.52887429	-1.18572554
6	1.28025183	-0.98359557	-0.66654044
6	2.49221782	-0.63388059	-1.27579135
6	2.52312712	0.22740729	-2.38436308
6	1.28844352	0.71299008	-2.88940525
6	0.08446794	0.35743711	-2.30150491
6	0.24421340	0.07694879	2.15220195
8	0.52167575	-0.41958942	3.18047445
8	2.25005912	2.57189491	0.76397843
6	1.29211228	1.89857508	0.69761711

1	-2.19688100	1.04740436	-0.99670081
1	-4.22590995	0.62623729	0.35301819
1	-4.54135494	-1.55830601	1.50206381
1	-2.74838071	-3.29590660	1.38628364
1	-0.66554449	-2.86730711	0.13237593
1	1.29709756	-1.67242882	0.17724891
1	3.42693188	-1.01220412	-0.85755847
7	3.71548956	0.56409641	-3.00780647
1	1.28719086	1.37774664	-3.75584104
1	-0.84427547	0.72966595	-2.73726565
8	-1.71368034	2.84423343	2.18533237
1	3.70810007	1.42030920	-3.55278471
1	4.55555188	0.46055483	-2.44751688

1-TS2

E = -236.331434 E0 = -236.113421

24	0.20041222	0.88901373	0.47901345
6	-0.64667978	2.44059347	0.87129933
6	-1.44426863	-1.08080533	-0.45858936
6	-2.54158302	-0.19677608	-0.32822278
6	-3.71486869	-0.60308190	0.31930695
6	-3.82731298	-1.89802002	0.82937799
6	-2.75601701	-2.79329061	0.68549054
6	-1.58042273	-2.39152893	0.05525505
6	-0.17450744	-0.62807266	-1.08680524
6	1.07876218	-1.20757296	-0.74216859
6	2.28141005	-0.75151587	-1.30169391
6	2.30757704	0.37738392	-2.14190323
6	1.07525424	1.02693141	-2.40579465
6	-0.13954564	0.51997277	-1.93277888
6	0.04122131	0.44567692	2.22691250

8	-0.05868326	0.16509410	3.36216308
8	2.77559706	2.24174635	1.11873854
6	1.75660140	1.71135030	0.86759251
1	-2.48217681	0.82028251	-0.71584390
1	-4.53760969	0.10464752	0.42869829
1	-4.74188844	-2.21352820	1.33323445
1	-2.84046972	-3.81156516	1.06826744
1	-0.76663695	-3.10842194	-0.05992504
1	1.11193354	-2.04501593	-0.04601545
1	3.21607902	-1.24494832	-1.02755719
7	3.48821858	0.84339661	-2.69900178
1	1.06554009	1.92492031	-3.02767201
1	-1.06568190	0.99482871	-2.25408779
8	-1.19023501	3.45051567	1.12602525
1	3.49014542	1.81798952	-2.98418797
1	4.34178193	0.57636805	-2.21817596

2

E = -236.383984 E0 = -236.164208

24	-1.09395695	-0.01980588	2.00511716
6	-0.60016529	1.74660527	2.13695553
6	-0.66628330	-0.45786827	-0.16744096
6	-1.79570717	0.40392819	-0.03764717
6	-2.93926576	0.03840433	0.71655352
6	-2.99122945	-1.21804847	1.38738279
6	-1.83148532	-2.04334685	1.35584044
6	-0.69355028	-1.65912049	0.60061213
6	0.48971276	-0.10348491	-1.02931373
6	1.81277760	-0.41128129	-0.65601426
6	2.88125206	-0.09300520	-1.49776518
6	2.65145825	0.54264354	-2.72504292

6	1.34177261	0.85575214	-3.10479624
6	0.26990376	0.53340823	-2.26596428
6	-1.89372818	0.11109476	3.65403447
8	-2.43156754	0.17433027	4.69115179
8	1.50938038	-0.66205404	3.36391936
6	0.49152787	-0.41524150	2.84344349
1	-1.77663215	1.38143297	-0.51851004
1	-3.77738311	0.73017781	0.79618395
7	-4.13893789	-1.62639034	2.04493831
1	-1.81404992	-2.97577540	1.91941142
1	0.17249170	-2.32016331	0.58765984
1	2.01153044	-0.86465526	0.31670384
1	3.90038885	-0.32651568	-1.18502659
1	1.15062001	1.34695652	-4.06041658
1	-0.74973879	0.75743851	-2.58547922
8	-0.27595754	2.86598455	2.21585267
1	3.48841207	0.79557151	-3.37765166
1	-3.99712514	-2.31169841	2.78215165
1	-4.76111799	-0.87822634	2.33879042

3a → 4b

3a

E = -236.379557 E0 = -236.159791

24	-1.10066244	-0.08413751	2.05429878
6	-0.04965315	1.42957061	2.10816318
6	-0.72198562	-0.38820663	-0.15819848
6	-1.83361388	0.50097378	0.05211841
6	-2.94131608	0.11363329	0.83879310
6	-2.94923132	-1.16010283	1.48201618
6	-1.85269555	-2.03353137	1.31794280
6	-0.74460904	-1.64313527	0.50797828

6	0.42295492	-0.00453164	-1.02989461
6	1.74479844	-0.10181456	-0.55898183
6	2.83570232	0.23747594	-1.36046425
6	2.60657855	0.68807646	-2.66718817
6	1.30603308	0.78148376	-3.15999243
6	0.19641898	0.43262368	-2.36330070
6	-1.94357663	0.53684016	3.56838849
8	-2.48444535	0.92672300	4.52638676
8	0.92262923	-1.40128419	3.85237236
6	0.13549671	-0.88911499	3.15885897
1	-1.80578537	1.49471675	-0.39294617
1	-3.75745734	0.81473630	1.00683099
1	-3.77653516	-1.43780468	2.13340975
1	-1.82938382	-2.98710492	1.84320428
1	0.10987852	-2.31140432	0.40354308
1	1.90416772	-0.42066617	0.47297780
1	3.84908353	0.16928025	-0.96480050
1	3.44440611	0.96797063	-3.30802982
1	1.13392560	1.12420588	-4.18336291
7	-1.09765876	0.55838068	-2.88490390
8	0.61621455	2.38624487	2.14032837
1	-1.13596720	0.57354649	-3.90005284
1	-1.78909102	-0.07455427	-2.49194487

3-TS1'

E = -236.323750 E0 = -236.106253

24	-0.26125232	0.37372579	1.75421115
6	0.24826798	2.11414787	1.74219817
6	-0.78420696	-0.58794989	-0.19829724
6	-1.97246165	0.19282613	-0.09026636
6	-3.07960884	-0.26512954	0.65963592

6	-2.98603423	-1.42610346	1.42502561
6	-1.74766976	-2.09700766	1.48566860
6	-0.67793502	-1.73337706	0.64853897
6	0.38246553	-0.15131851	-1.00953671
6	1.67666171	-0.26918012	-0.45141292
6	2.81137578	0.21907525	-1.09972228
6	2.66421321	0.81208476	-2.35906393
6	1.40857376	0.89401299	-2.95938237
6	0.24976664	0.41498451	-2.31445365
6	-1.35614946	0.74718611	3.14007560
8	-2.06234605	0.99291814	4.04392954
8	1.88014445	-0.12203034	3.77898626
6	1.04580548	0.06891703	2.97616920
1	-2.04357114	1.14296953	-0.62084492
1	-3.99570300	0.32770482	0.66910723
1	-3.82516596	-1.76327333	2.03237348
1	-1.62732913	-2.95721992	2.14608479
1	0.21605195	-2.35544825	0.60880712
1	1.78856263	-0.73665898	0.53115910
1	3.78913275	0.14274525	-0.62547689
1	3.53522966	1.20336936	-2.88729190
1	1.31219018	1.32408042	-3.95907121
7	-0.95346285	0.40941449	-3.00500363
8	0.57687661	3.23980424	1.74457353
1	-1.04268289	1.05390805	-3.78166395
1	-1.80809384	0.24490390	-2.48899942

3-IM

E = -236.334163 E0 = -236.116305

24	0.00929797	0.92318360	1.06872770
----	------------	------------	------------

6	-0.99113867	2.04604980	2.10293410
---	-------------	------------	------------

6	-0.97081041	-0.73998771	-0.11795327
6	-1.97922772	0.26647961	0.05417289
6	-3.19842937	-0.04741038	0.70558719
6	-3.40190870	-1.31368772	1.23092258
6	-2.39594526	-2.29995123	1.11149932
6	-1.20246200	-2.01863045	0.46331914
6	0.32277780	-0.36459577	-0.74119755
6	1.53833433	-0.74133089	-0.08480223
6	2.79174833	-0.34661694	-0.58170799
6	2.85236305	0.46723743	-1.71141810
6	1.68370231	0.84183724	-2.38468734
6	0.41549391	0.41417657	-1.95107302
6	0.46539971	0.13110654	2.62244520
8	0.75185236	-0.38951276	3.63502296
8	2.29218298	2.84962652	1.33823054
6	1.40408895	2.09548540	1.23495240
1	-1.89626512	1.23387545	-0.45889474
1	-3.96450193	0.72271937	0.80265023
1	-4.33382151	-1.54735179	1.74685968
1	-2.55718104	-3.29219827	1.53499560
1	-0.43738145	-2.79021716	0.36533013
1	1.48971223	-1.43212508	0.75591346
1	3.70024956	-0.66239793	-0.06998248
1	3.81643093	0.80891036	-2.09054523
1	1.75225536	1.43531906	-3.29909506
7	-0.69514672	0.63409099	-2.74292321
8	-1.62906107	2.75790251	2.78012949
1	-0.65912604	1.39240542	-3.41361866
1	-1.61183753	0.41968977	-2.36973684

3-TS2'

E = -236.323700 E0 = -236.105611

24	0.40180056	1.03575555	1.08651052
6	-0.65008022	2.37658836	1.68972593
6	-1.23964693	-0.97840384	-0.15378852
6	-2.32242161	-0.14303743	0.20398944
6	-3.51048263	-0.68761128	0.70762425
6	-3.64727234	-2.07163848	0.84399492
6	-2.58564220	-2.91241938	0.48187856
6	-1.39365398	-2.37309436	-0.00475013
6	0.06829599	-0.41910784	-0.61502394
6	1.27398011	-0.95516564	-0.06659499
6	2.53222300	-0.48698666	-0.46828606
6	2.61852328	0.52254682	-1.43924945
6	1.45744165	1.07312240	-1.97817435
6	0.16682350	0.60216376	-1.62025554
6	0.59449919	0.51234200	2.80431995
8	0.73407199	0.17898718	3.92141465
8	2.73220694	2.84376343	1.47240513
6	1.81146134	2.13083381	1.31957743
1	-2.22507733	0.94355450	0.13488666
1	-4.32269504	-0.02234802	1.00348001
1	-4.57408021	-2.49538078	1.23326339
1	-2.68690178	-3.99431608	0.58094047
1	-0.57599972	-3.03642624	-0.29096815
1	1.19972197	-1.75674312	0.66834093
1	3.43307622	-0.90263431	-0.01717115
1	3.59012929	0.90985004	-1.74587347
1	1.53046008	1.85670588	-2.73567213
7	-0.93802456	1.03137828	-2.33547329
8	-1.33518256	3.24947903	2.08167773
1	-0.87082242	1.94549231	-2.77013142

1 -1.85211104 0.82183931 -1.94906727

4b

E = -236.383232 E0 = -236.163297

24 -0.58264363 0.17882713 1.67225110
6 0.17231841 1.85092093 1.81214633
6 -0.16281858 -0.20884783 -0.53475261
6 -1.24462625 0.70990452 -0.36213091
6 -2.39420455 0.38745054 0.39521250
6 -2.42760630 -0.85717045 1.07812962
6 -1.36983241 -1.78434031 0.93196365
6 -0.25513560 -1.50017302 0.08221713
6 0.98647920 0.14063535 -1.42214114
6 2.29966208 0.26354301 -0.92882098
6 3.35483869 0.57802212 -1.79277824
6 3.11393347 0.78146110 -3.15696117
6 1.81044778 0.66995753 -3.65463039
6 0.75440413 0.34882237 -2.79478115
6 -1.34350345 0.48821577 3.31441794
8 -1.83076629 0.69155016 4.35730217
8 1.81851858 -0.99467208 3.04932971
6 0.88247603 -0.52056556 2.52873930
1 -1.15859733 1.69307319 -0.82477782
1 -3.19096733 1.11636719 0.52844858
1 -1.40242912 -2.73299139 1.46742788
7 0.69715263 -2.46979471 -0.15548751
1 2.48189552 0.14829686 0.14163737
1 4.36503802 0.68329770 -1.39355664
1 1.61323944 0.83128292 -4.71579916
1 -0.25951504 0.25065562 -3.18800376
8 0.65344940 2.91169198 1.90282701

1 3.93704192 1.03407012 -3.82714134
1 -3.26345577 -1.10090801 1.73246097
1 1.58494166 -2.13359068 -0.52045256
1 0.79976979 -3.18096946 0.56198642

3b → 4a

3b

E = -236.379043 E0 = -236.158812

24 -0.75045439 -0.04410796 1.99245458
6 0.44816698 1.33379717 2.19119644
6 -0.42470867 -0.36636152 -0.28237202
6 -1.54415161 0.50338845 -0.04467261
6 -2.61084561 0.11023682 0.79044209
6 -2.59434708 -1.15741214 1.44303103
6 -1.48155088 -2.00341286 1.26249936
6 -0.40115250 -1.60174446 0.42350077
6 0.62137941 -0.06622995 -1.29507273
6 1.11236317 -1.14611661 -2.06111612
6 2.04606772 -0.97643231 -3.08185807
6 2.51675766 0.31325800 -3.36164058
6 2.05386123 1.39842345 -2.62310024
6 1.11076523 1.24162932 -1.58449379
6 -1.62927889 0.69291176 3.42790710
8 -2.19625062 1.15556299 4.33763823
8 1.00073076 -1.53499860 3.92955989
6 0.32266014 -0.95160756 3.18050063
1 -1.58459339 1.47391230 -0.53586969
1 -3.43962209 0.79682177 0.95806741
1 -3.40323293 -1.44332691 2.11308553
1 -1.42162130 -2.94836520 1.80083741
1 0.47227792 -2.24621554 0.33998795

1	0.71335946	-2.14364997	-1.87049815
1	2.39122773	-1.83477408	-3.65826063
1	3.24755693	0.47480424	-4.15581216
1	2.42960769	2.40197338	-2.83727324
7	0.66304016	2.37398218	-0.90503001
8	1.20998146	2.20359275	2.38533514
1	1.27721175	3.17829802	-1.00241414
1	0.41042855	2.22481719	0.06962215

3-TS1

E = -236.329368 E0 = -236.110882

24	0.36896750	0.78218742	1.52980732
6	2.08809799	1.23210201	1.92564172
6	-0.20637402	-0.50672986	-0.68926978
6	-1.21119667	0.32678281	-0.10796925
6	-1.86934108	-0.07322689	1.08033272
6	-1.52661102	-1.29432990	1.69458244
6	-0.50589936	-2.08906057	1.16468113
6	0.16392094	-1.67990903	-0.00779493
6	0.53875976	-0.11033555	-1.90691542
6	0.69376967	-0.99937445	-2.98547365
6	1.50414694	-0.67231503	-4.07608524
6	2.18868900	0.54936211	-4.08986431
6	2.04113999	1.44554047	-3.02722043
6	1.20883207	1.13644590	-1.94030156
6	-0.05072320	2.47065873	1.96668527
8	-0.31709643	3.58179444	2.25461125
8	0.07622590	0.16429356	4.43454855
6	0.17437946	0.38249374	3.28472051
1	-1.56804855	1.20679349	-0.64316305
1	-2.67011349	0.54114700	1.49017688

1	-2.02401626	-1.58669659	2.61977069
1	-0.19667039	-2.99974768	1.67745444
1	0.98676911	-2.27956784	-0.40050722
1	0.16941037	-1.95678147	-2.96172743
1	1.60708455	-1.37061277	-4.90753573
1	2.83301727	0.80970248	-4.93096562
1	2.57510929	2.39862969	-3.03583104
7	1.11389092	1.98284732	-0.79637949
8	3.17957884	1.56442892	2.19767666
1	1.91083106	2.61319287	-0.70638249
1	0.26034896	2.53836305	-0.75651138

3-IM1

E = -236.340093 E0 = -236.120303

24	0.52062657	1.05232389	1.33677663
6	2.18127389	1.56944987	1.87565674
6	-0.28925369	-0.61435820	-0.62639953
6	-1.19333208	0.31747721	-0.03103595
6	-1.86579215	-0.03186840	1.16016763
6	-1.81096548	-1.36265510	1.64199644
6	-0.97915508	-2.28702906	1.02565245
6	-0.17103201	-1.89400428	-0.06312651
6	0.54295818	-0.20901066	-1.78275427
6	0.78020750	-1.08549006	-2.85953035
6	1.62007178	-0.72435818	-3.91491247
6	2.24813006	0.52703472	-3.91049912
6	2.01787994	1.41373003	-2.85446995
6	1.16466264	1.06030680	-1.80192826
6	-0.11199448	2.52848050	2.14300692
8	-0.53416423	3.49318175	2.67231538
8	0.39962799	-0.33865324	3.98937962

6	0.41712683	0.18874136	2.94142123
1	-1.47202201	1.23040779	-0.55774019
1	-2.54675270	0.68416483	1.62021793
1	-2.39261339	-1.64108660	2.52107673
1	-0.90189063	-3.30293982	1.41447664
1	0.55861429	-2.59284393	-0.47645096
1	0.28536889	-2.05818735	-2.86580912
1	1.78596506	-1.41900119	-4.73932153
1	2.91318390	0.81520969	-4.72554281
1	2.50995845	2.38927266	-2.84221826
7	0.98203594	1.95683899	-0.66956079
8	3.23826163	1.91133915	2.25785351
1	1.80947586	2.54860894	-0.56655230
1	0.19938036	2.59703386	-0.83367143

3-TS2

E = -236.338820 E0 = -236.119009

24	0.88722151	1.03958686	1.00143098
6	2.46603844	1.77981356	1.51349432
6	-0.36091389	-0.43940801	-0.44836716
6	-1.35409461	0.44170083	0.06962566
6	-2.25263599	-0.00701930	1.06440094
6	-2.19940060	-1.31129297	1.54083402
6	-1.22865414	-2.19728246	1.03340960
6	-0.32025186	-1.76636003	0.07719364
6	0.53745326	-0.09222525	-1.59017222
6	0.92266442	-1.08860557	-2.51539710
6	1.82742619	-0.82712746	-3.54393638
6	2.38809629	0.44937469	-3.67857544
6	2.01098771	1.46016709	-2.79359191
6	1.08799909	1.20376720	-1.77075417

6	0.07380540	2.09531928	2.21090471
8	-0.46059359	2.77819352	3.00638857
8	1.29834099	-0.92738267	3.22591674
6	1.12779286	-0.17576398	2.33999773
1	-1.57371942	1.39335110	-0.41197678
1	-3.00243284	0.68758923	1.44548112
1	-2.89473830	-1.64203365	2.31273685
1	-1.16021539	-3.21396721	1.42184717
1	0.46404195	-2.44429037	-0.26127684
1	0.48395530	-2.08304825	-2.43038075
1	2.09703971	-1.62144740	-4.24103520
1	3.10856321	0.65890414	-4.46991750
1	2.43633819	2.46182785	-2.88839528
7	0.75201800	2.22854143	-0.80846187
8	3.48059962	2.25387214	1.87072141
1	1.43349697	2.98865342	-0.82769066
1	-0.17038667	2.63870822	-0.97598016

3-IM2

E = -236.342713 E0 = -236.123008

24	0.98466571	1.10363901	0.56158494
6	2.64046316	1.84934231	0.70600072
6	-0.50684280	-0.39007822	-0.41207264
6	-1.42959585	0.53746462	0.16197188
6	-2.34513470	0.12724342	1.16427676
6	-2.36786804	-1.17749922	1.62153043
6	-1.46352010	-2.11220222	1.06761135
6	-0.55902647	-1.73100922	0.09563966
6	0.50580755	-0.04265737	-1.44504840
6	1.15661635	-1.08145803	-2.17972463
6	2.18323417	-0.84086626	-3.07436343

6	2.64722605	0.47408569	-3.29000362
6	2.03732347	1.52125851	-2.62626937
6	0.96932217	1.29566896	-1.72205913
6	0.48604837	2.00689056	2.06753924
8	0.16581854	2.59254740	3.03008871
8	2.12637394	-1.07786625	2.27524757
6	1.66230432	-0.23643842	1.60380170
1	-1.62768049	1.50816993	-0.27925338
1	-3.04313597	0.86512575	1.56216090
1	-3.06811353	-1.48190650	2.39986903
1	-1.45263258	-3.14069888	1.43102127
1	0.16622399	-2.46448896	-0.25205461
1	0.80190866	-2.10359417	-2.06030462
1	2.63198189	-1.67485674	-3.61496769
1	3.46933507	0.66720500	-3.97946931
1	2.36569895	2.54944796	-2.79338210
7	0.37305968	2.40795596	-1.04376830
8	3.71444552	2.30752284	0.82353345
1	0.91604161	3.26290613	-1.16025315
1	-0.60346953	2.58722478	-1.28809167

3-TS3

E = -236.341380 E0 = -236.121804

24	1.04601955	1.08073552	0.58306539
6	2.66522857	1.88308298	0.68656665
6	-0.58955039	-0.37809280	-0.41604994
6	-1.69946527	0.45739241	-0.13063753
6	-2.68265882	0.07741387	0.79939396
6	-2.59141164	-1.14086650	1.46653843
6	-1.49750430	-1.98525567	1.21050919
6	-0.51317303	-1.60581926	0.30572927

6	0.48286130	-0.04440806	-1.39439362
6	1.16504724	-1.09160940	-2.08212630
6	2.19334318	-0.84664803	-2.97577925
6	2.61092080	0.47647688	-3.23280638
6	1.97573868	1.52912190	-2.59828014
6	0.91658975	1.29867738	-1.68596812
6	0.56396271	1.93692674	2.12089395
8	0.25932676	2.49772606	3.10393195
8	2.38132226	-1.06759322	2.19684397
6	1.83064989	-0.24734464	1.56303405
1	-1.89303376	1.35724829	-0.71058048
1	-3.52240567	0.74762857	0.98648079
1	-3.35217580	-1.42999053	2.19259128
1	-1.39391442	-2.92762761	1.74943054
1	0.35451660	-2.24945562	0.16598601
1	0.83383477	-2.11719956	-1.92008832
1	2.67948009	-1.68141838	-3.48145073
1	3.42912981	0.67289090	-3.92608244
1	2.28701359	2.55871526	-2.78723041
7	0.33042781	2.39320494	-0.97144223
8	3.72492064	2.38449174	0.77156217
1	0.86049983	3.25645679	-1.08290247
1	-0.65869138	2.56834956	-1.14524521

3-IM3

E = -236.345765 E0 = -236.126180

24	1.21916944	0.80870016	0.59372797
6	2.73904223	1.79858547	0.70015048
6	-0.63925702	-0.34863282	-0.44098836
6	-1.89316933	0.30987592	-0.58520761
6	-2.91412932	0.12232352	0.33773873

6	-2.72342680	-0.73344978	1.44126657
6	-1.52623564	-1.42706107	1.57764200
6	-0.48494591	-1.25536637	0.64203702
6	0.48610864	-0.09867963	-1.38248884
6	1.16839242	-1.12291830	-2.09367097
6	2.17527220	-0.81682299	-2.99703983
6	2.54722454	0.52689121	-3.22387863
6	1.91944070	1.55592547	-2.53754111
6	0.89563327	1.25991102	-1.60702487
6	0.76101552	1.41460574	2.25632930
8	0.45983737	1.81241568	3.31634607
8	3.00504583	-1.31976515	1.72801288
6	2.27348997	-0.51259558	1.28991304
1	-2.07521705	0.92932235	-1.46773391
1	-3.86857945	0.63298523	0.20153585
1	-3.52207373	-0.86689164	2.17210561
1	-1.38403165	-2.12134071	2.40674752
1	0.39288614	-1.89426603	0.69809784
1	0.86733509	-2.15917406	-1.93190641
1	2.68702040	-1.61881283	-3.52967228
1	3.34503024	0.75948664	-3.92986942
1	2.21926614	2.59411917	-2.69331617
7	0.30344883	2.24778554	-0.76042770
8	3.73850596	2.40789901	0.79196635
1	0.73948711	3.16491143	-0.83159848
1	-0.71473675	2.31324390	-0.77975861

3-TS4

E = -236.338710 E0 = -236.119324

24	1.76858251	0.98503651	0.39009600
6	3.20293950	2.06220573	0.51852877

6	-0.84210065	-0.37366494	-0.48087370
6	-2.07161195	0.30435428	-0.62643489
6	-3.12191253	0.07155480	0.26621838
6	-2.96157204	-0.83836881	1.31972150
6	-1.75145837	-1.52449085	1.46644810
6	-0.69828787	-1.29954207	0.57242144
6	0.29204556	-0.12557780	-1.41952376
6	0.85395661	-1.17441083	-2.18078328
6	1.93328646	-0.95516199	-3.03824853
6	2.51061960	0.31801909	-3.11588601
6	1.98135073	1.38250875	-2.37492929
6	0.82216608	1.19238307	-1.58786559
6	1.39512132	1.39681561	2.11532608
8	1.15830074	1.67224140	3.23195846
8	3.52722853	-1.27916263	1.27084511
6	2.83375385	-0.39686736	0.92537342
1	-2.21985505	0.98294284	-1.47077207
1	-4.07001680	0.59555568	0.13495428
1	-3.77840373	-1.01141260	2.02171499
1	-1.61737328	-2.22965267	2.28784498
1	0.25058994	-1.82273758	0.70084691
1	0.42495147	-2.17232120	-2.07941576
1	2.34925153	-1.78331364	-3.61196119
1	3.38708367	0.49001558	-3.74094004
1	2.43200753	2.37430890	-2.43260228
7	0.39121673	2.23524572	-0.72013615
8	4.14494838	2.76288797	0.60755859
1	0.70016589	3.16957727	-0.97887226
1	-0.58999414	2.20768361	-0.44314020

3-IM4

E = -236.340847 E0 = -236.121497

24	2.11415964	1.09840875	0.23554849
6	3.31773176	2.42125862	0.47242397
6	-0.96085608	-0.38939131	-0.42239255
6	-2.14757454	0.33811656	-0.65084672
6	-3.28191274	0.11748375	0.13893231
6	-3.25007431	-0.83354610	1.16517352
6	-2.07910757	-1.56711396	1.39430943
6	-0.94314292	-1.34740875	0.60998059
6	0.24336748	-0.16596519	-1.27266401
6	0.83519009	-1.23123038	-1.97918834
6	1.93313765	-1.04336336	-2.82773112
6	2.49305490	0.22931287	-2.95638286
6	1.95425694	1.32481829	-2.25927180
6	0.79932692	1.14271514	-1.44990368
6	1.79505620	1.15279171	2.02347541
8	1.58646394	1.19162027	3.17807222
8	4.28840211	-0.92854743	0.63649401
6	3.43737725	-0.13567922	0.48228701
1	-2.19518378	1.05081113	-1.47812519
1	-4.19474295	0.68248221	-0.05690941
1	-4.13263106	-1.00202388	1.78381679
1	-2.04350686	-2.30260090	2.19936098
1	-0.02201554	-1.89608166	0.81423209
1	0.39824545	-2.22530772	-1.86841095
1	2.36141403	-1.89158486	-3.36069869
1	3.36100198	0.38791165	-3.59762211
1	2.36903139	2.32353953	-2.39874293
7	0.41339609	2.19745882	-0.58251914
8	4.10347911	3.28430663	0.61790519
1	0.58527413	3.14238831	-0.91890996

1 -0.50163850 2.09107233 -0.14422054

3-TS5

E = -236.331278 E0 = -236.113795

24 2.21788435 0.98212725 0.06675193
6 3.31481653 2.35712905 0.48409621
6 -0.99271332 -0.29743086 -0.31212946
6 -2.21504803 0.30597321 -0.67277068
6 -3.38215758 0.03944355 0.05203771
6 -3.34946852 -0.83581140 1.14363202
6 -2.14130699 -1.44505743 1.50607231
6 -0.97316756 -1.17785124 0.78733862
6 0.23956802 -0.05063662 -1.11574634
6 0.98545622 -1.14117627 -1.63494840
6 2.09185943 -0.96669485 -2.47224427
6 2.53550943 0.33452396 -2.74445492
6 1.83291221 1.45466619 -2.25842166
6 0.66585591 1.27211440 -1.46461755
6 1.77755892 0.90076773 1.82230857
8 1.49030054 0.85915829 2.96024406
8 4.48067040 -0.88449815 0.61424835
6 3.59065423 -0.15323567 0.39486329
1 -2.25703874 0.96800847 -1.54027475
1 -4.32085588 0.50965044 -0.24583073
1 -4.25907982 -1.04059271 1.71016543
1 -2.10404380 -2.12033087 2.36223350
1 -0.02860052 -1.63097126 1.09314249
1 0.64989240 -2.14855010 -1.38193255
1 2.64124264 -1.82973259 -2.84501969
1 3.43069936 0.49825187 -3.34563625
1 2.15918346 2.46334058 -2.51329710

7	0.09801699	2.37709634	-0.84821682
8	4.02373799	3.25383019	0.75628671
1	0.57155626	3.27143436	-0.89280630
1	-0.57704512	2.23826465	-0.10357972

4a

E = -236.383480 E0 = -236.163516

24	-1.04225763	0.32923978	1.70442087
6	-0.76706163	2.14172129	1.78514219
6	-0.44523280	-0.26563066	-0.41951756
6	-1.61398945	0.55291827	-0.40355303
6	-2.77810847	0.19424068	0.32269235
6	-2.73412467	-0.96120860	1.13867937
6	-1.58121291	-1.78691517	1.16086899
6	-0.44655179	-1.47825554	0.35516032
6	0.71391138	0.10574249	-1.28518279
6	1.12074472	-0.76487016	-2.31629105
6	2.17191213	-0.41280385	-3.17050562
6	2.82686300	0.81386748	-3.01235469
6	2.42647681	1.68635075	-1.99271821
6	1.38147282	1.33530234	-1.13213642
6	-1.80681415	0.47957540	3.36946784
8	-2.29841674	0.57963872	4.42453751
8	1.63832548	-0.09308847	3.00004071
6	0.59045792	0.08546589	2.51154006
1	-1.60243203	1.47248161	-0.98837202
1	-3.65130770	0.84334442	0.32202652
1	-1.55497336	-2.66465164	1.80611050
7	0.63401859	-2.34033469	0.32478889
1	0.60263224	-1.71562606	-2.45553423
1	2.47206479	-1.09635071	-3.96657774

1	2.93687090	2.64136353	-1.85733980
1	1.08850918	2.00614557	-0.32294343
8	-0.59663463	3.29813201	1.84033049
1	3.64688888	1.08758955	-3.67808271
1	-3.58471854	-1.21780811	1.76882958
1	0.74083439	-2.93193093	1.14405486
1	1.51185555	-1.92364384	0.02241915

Rotation

3-TS(rot)

E = -236.368165 E0 = -236.148009

24	-0.79668894	0.05352119	1.90747698
6	-0.66357014	1.86551737	2.22512369
6	-0.56679125	-0.44178093	-0.32264337
6	-1.61671035	0.50089095	-0.10368978
6	-2.70219573	0.24647603	0.78716630
6	-2.74910900	-0.94650236	1.53351325
6	-1.70327598	-1.89830127	1.37455365
6	-0.62741903	-1.62829893	0.50250185
6	0.57886362	-0.25284300	-1.26096344
6	1.42354995	-1.36190930	-1.51192388
6	2.59896652	-1.27840864	-2.25360087
6	2.98136641	-0.04448405	-2.79006631
6	2.13988053	1.05149413	-2.62828582
6	0.92862560	0.97333988	-1.91089858
6	-1.06289356	-0.17572696	3.71373664
8	-1.23641503	-0.32472303	4.85890662
8	2.16227015	-0.14798237	2.42199003
6	1.01498709	-0.06712297	2.22701823
1	-1.58509713	1.47840690	-0.56758574
1	-3.46027307	1.01469883	0.93144793

1	-3.54873050	-1.11862841	2.25229250
1	-1.68560526	-2.80108878	1.98318862
1	0.19162692	-2.34120728	0.48761534
1	1.15305768	-2.33818909	-1.11407461
1	3.21146847	-2.16775836	-2.40326519
1	3.90843591	0.05813424	-3.35576526
1	2.40362664	2.00777155	-3.08801835
7	0.14917104	2.14544757	-1.82808230
8	-0.58644788	3.01279086	2.42193652
1	0.56194021	2.90560144	-2.36610032
1	-0.81661683	2.02086250	-2.12350830

4-TS(rot)

E = -236.369838 E0 = -236.149751

24	-0.89930309	0.17989222	1.82266580
6	-0.06660712	1.81542684	1.98080187
6	-0.42596096	-0.20337916	-0.42573580
6	-1.48386508	0.75108260	-0.20221225
6	-2.66933134	0.47686917	0.51158050
6	-2.79194984	-0.77290857	1.16543696
6	-1.75801175	-1.72029736	1.03352454
6	-0.58176887	-1.47046713	0.25194668
6	0.68835385	0.17650874	-1.35315444
6	0.58822102	1.36989284	-2.11171546
6	1.58992623	1.78094091	-2.99182618
6	2.74303857	1.01023491	-3.16835511
6	2.85688086	-0.18638371	-2.45829258
6	1.85439745	-0.59524850	-1.57311879
6	-1.69777211	0.52226741	3.44080884
8	-2.20782105	0.74645293	4.46771256
8	1.40800616	-1.10457524	3.25983488

6	0.50717883	-0.58453616	2.72378007
1	-1.37848681	1.75063482	-0.61183158
1	-3.42454548	1.25074393	0.63383340
1	-1.82566752	-2.66620250	1.57158240
7	0.33324937	-2.52347511	0.17006307
1	-0.29438242	2.00196525	-2.04343004
1	1.45981789	2.71158939	-3.54662944
1	3.73620919	-0.81978085	-2.58654039
1	2.00653760	-1.55393173	-1.09319036
8	0.45642937	2.85472354	2.07475518
1	3.52955623	1.33061485	-3.85271037
1	-3.65558210	-0.99488540	1.79046771
1	1.30363786	-2.25471894	0.30844184
1	0.09961625	-3.27905115	0.81150763