

Meeting the Challenge of Magnetic Coupling in a Triply-Bridged Chromium Dimer: Complementary Broken-Symmetry DFT and Multireference DMRG Perspectives

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SUPPORTING INFORMATION

Table S1. Total energies (in a.u.), spin expectation values from high-spin (HS) and broken-symmetry (BS) solutions, and exchange coupling constants (in cm^{-1}) obtained with different functionals at the reference geometry.

	TPSSh	B3LYP	TPSS0	PBE0
E_{HS}	-3356.12584162	-3355.04313221	-3355.88952760	-3354.08625140
E_{BS}	-3356.12933925	-3355.04619247	-3355.89205143	-3354.08899452
$\langle S^2 \rangle_{\text{HS}}$	12.0411	12.0461	12.0433	12.0550
$\langle S^2 \rangle_{\text{BS}}$	2.9883	3.0095	3.0172	3.0261
J	-84.8	-74.3	-61.4	-66.7

	TPSS	PBE	BP86	BLYP
E_{HS}	-3356.29483182	-3353.91375443	-3356.29358239	-3355.46227976
E_{BS}	-3356.29954967	-3353.91906773	-3356.29877648	-3355.46780851
$\langle S^2 \rangle_{\text{HS}}$	12.0380	12.0517	12.0524	12.0410
$\langle S^2 \rangle_{\text{BS}}$	2.9425	2.9344	2.9389	2.9189
J	-113.8	-127.9	-125.1	-133.0

Table S2. Important structural parameters (Cr–Cr distance, average Cr–O(H) bond length, Cr–O(H)–Cr angle) from fully optimized broken-symmetry geometries with different functionals, including D3BJ corrections, and the corresponding exchange coupling constants J .

	Cr–Cr (\AA)	Cr–O (\AA)	Cr–O–Cr ($^\circ$)	J (cm^{-1})
TPSS	2.695	2.005	84.4	-88.2
PBE	2.699	2.013	84.2	-96.7
TPSSh	2.708	1.999	85.2	-56.0
TPSS0	2.709	1.991	85.7	-38.0
B3LYP	2.731	2.010	85.6	-43.6

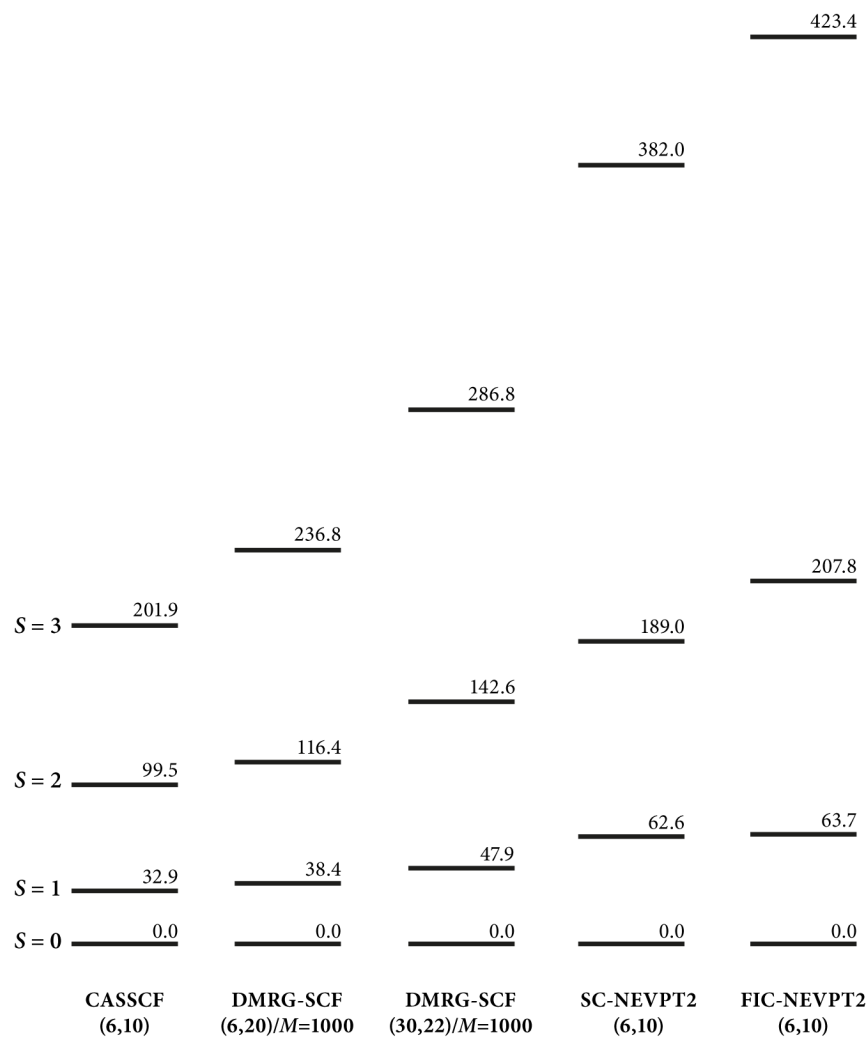


Figure S1. Spin ladders produced by different wave function based methods for the dinuclear chromium complex under investigation.

Cartesian coordinates of all models

TPSS H-only optimized model

Cr	-1.32077675789660	0.00004567211811	-0.00007096467317
Cr	1.32077324283384	0.00005158303881	-0.00007157859457
O	-0.00000104868858	-0.16583237580723	1.45467585745211
O	-0.00000489764937	1.34277292975137	-0.58371627199903
O	0.00000067419445	-1.17682896850597	-0.87101026120097
H	0.00001790208267	0.50127981586150	2.15993328303163
H	0.00056213619050	1.61869136067886	-1.51448427772977
H	-0.00044104651121	-2.12078532888951	-0.64413286649204
N	-2.64979639176962	-1.44569378219198	0.71141991748241
C	-1.96723877683042	-2.53150336334491	1.49741316302721
C	-3.24368037350626	-2.03126564893063	-0.53390524471276
C	-3.70971767634131	-0.79482652965216	1.56203025179475
H	-1.50611109500905	-2.09494287212245	2.38227714666532
H	-1.20003332072637	-2.99746593446751	0.87727778775072
H	-2.69709429184401	-3.29417670409302	1.78680599374014
H	-2.45713087989536	-2.63082378918971	-1.00368039677010
H	-4.06474101618296	-2.71373529840676	-0.28162892858883
H	-4.62553838458745	-0.71938852428422	0.97193419906511
H	-3.94180643056544	-1.43233893352354	2.41956824499303
N	-2.64980256138524	1.33901556828090	0.89630056028452
N	-2.64980038336441	0.10677232402498	-1.60776835378432
C	-3.70971800240785	-0.95531484258297	-1.46940407035238
C	-3.24368562009935	0.55331550766570	2.02608271830195
N	2.64980067794514	-1.44568193229971	0.71141868600201
N	2.64979447720107	1.33902743110622	0.89629932793762
N	2.64979663544791	0.10678418068707	-1.60776957870374
C	-1.96725035879470	2.56261235577474	1.44364406188149
C	-3.70972375060080	1.75022808457439	-0.09267425723559
C	-1.96724550946031	-0.03101115292470	-2.94110526383651
C	-3.24368848245842	1.47803937363856	-1.49222464129291
H	-4.62558984511764	-0.48221330653117	-1.10887816237189
H	-3.94175413156726	-1.37940439028017	-2.45019713433286
H	-2.45710023893015	0.44599637215694	2.78010888133082
H	-4.06480735461771	1.11280848002045	2.49108824409826
C	1.96724725554052	-2.53149455336756	1.49741224378802
C	3.24368569356644	-2.03125112915353	-0.53390676339270
C	3.70971844014110	-0.79480993568548	1.56202852714936
C	1.96723601210309	2.56262114404852	1.44364312933477
C	3.24368056139230	0.55333001361486	2.02608120711149
C	3.70971236083504	1.75024468234002	-0.09267599934625
C	1.96724081992101	-0.03100234186851	-2.94110620541212
C	3.24367767216167	1.47805387752771	-1.49222616709369
C	3.70971807894818	-0.95529823271254	-1.46940580237183
H	-1.50375290990065	3.10925190551415	0.62354092184389
H	-1.20171313853662	2.25877752450171	2.15909815420654
H	-2.69767375679224	3.19578710394873	1.95706724009970
H	-4.62543371684035	1.20116961382526	0.13681738047320
H	-3.94200796666106	2.81155859771218	0.03059305603763
H	-1.50276864801509	-1.01409155231681	-3.00420649677802

H	-1.20309418638945	0.74187206739252	-3.03572600131324
H	-2.69797575471462	0.09546145526857	-3.74614669451067
H	-2.45703697100368	2.18462404933411	-1.77634058940058
H	-4.06475178550869	1.60090730318433	-2.20935862370879
H	1.50614862542804	-2.09494317731569	2.38229660706312
H	1.20002265002298	-2.99741709798907	0.87727577268110
H	2.69710252932602	-3.29417828809696	1.78677807515430
H	2.45714267657494	-2.63082369046460	-1.00366709050502
H	4.06476961090010	-2.71369418770397	-0.28163224842656
H	4.62555565455524	-0.71940605121393	0.97195330268582
H	3.94178307498783	-1.43230113185123	2.41958979056064
H	1.50357479424781	3.10918222005415	0.62358103033223
H	1.20182998798639	2.25879076334749	2.15924302589083
H	2.69768680938841	3.19588061502689	1.95692445402491
H	2.45708429727129	0.44597962062585	2.78009130737457
H	4.06478059679567	1.11284184879546	2.49110060500510
H	4.62541221159885	1.20116314525263	0.13680039348052
H	3.94201224677884	2.81156990751106	0.03060321408914
H	1.50267872785295	-1.01404489669261	-3.00416424100455
H	1.20314783285142	0.74193593536788	-3.03579980829302
H	2.69798268801952	0.09538099720936	-3.74615088499019
H	2.45703083735398	2.18464798306617	-1.77634272668040
H	4.06473833125488	1.60093248495915	-2.20936143690374
H	4.62558786531673	-0.48219041570644	-1.10888361173207
H	3.94174955515341	-1.37938388964014	-2.45020164669110

TPSS fully optimized model

Cr	-1.34758593490855	0.00565339229796	-0.00096991259459
Cr	1.34758597894758	0.00565505923656	-0.00096912250690
O	-0.00000058681353	-0.14068912029890	1.47726606953343
O	0.00000049692156	1.36355074258827	-0.60745587477747
O	0.00000033154978	-1.19674421955831	-0.87215310122970
H	-0.00000147733120	0.53514405211360	2.17337951575592
H	0.00000555193572	1.63823989727589	-1.53798052909426
H	-0.00000294619366	-2.13958125763495	-0.64331167802615
N	-2.68355245059462	-1.46194843953389	0.70738154328941
C	-2.01669403937965	-2.53288674992317	1.51035253135120
C	-3.26270227964075	-2.05562375138987	-0.54717490101104
C	-3.75350669308604	-0.80186558590005	1.55369697655965
H	-1.56186335898789	-2.08767748464231	2.39477070334976
H	-1.24259377516028	-3.00990244641601	0.90659640658413
H	-2.75033756273477	-3.29070948673219	1.80363285556860
H	-2.46366827416375	-2.62917487932995	-1.02603961365256
H	-4.07529053743538	-2.75071519155338	-0.30444529949035
H	-4.65941540476408	-0.70398667333438	0.95425308132621
H	-4.00212852775245	-1.44894166869915	2.39913095898057
N	-2.69435793696765	1.34365691707395	0.91262843918709
N	-2.69085988683319	0.11818724803085	-1.62007504186865
C	-3.75419882415905	-0.95080721639590	-1.46720590196571
C	-3.27124097756576	0.54981108795692	2.05234215929801
N	2.68355198482338	-1.46194540404780	0.70738820877094
N	2.69435838650554	1.34366073992367	0.91262530213621
N	2.69086040986888	0.11818237772104	-1.62007335069977

C	-2.03672692173826	2.57868185896727	1.44091058784838
C	-3.76424890526605	1.73941765849069	-0.08510019994679
C	-2.02863953251995	-0.03691008284133	-2.95207500926779
C	-3.27683735349459	1.49836560289158	-1.50380470480896
H	-4.66138433817800	-0.48570720074034	-1.07951842417071
H	-4.00412182836442	-1.36130174943495	-2.44920091573159
H	-2.47293114884143	0.42590964548178	2.78996282389631
H	-4.08817164590353	1.10234421931994	2.53157594335328
C	2.01669446106521	-2.53288026946344	1.51036450795159
C	3.26270138788802	-2.05562545635176	-0.54716629492317
C	3.75350692436350	-0.80185953643050	1.55370058161288
C	2.03672670899738	2.57868691824845	1.44090381473139
C	3.27124152896244	0.54981867219544	2.05234154856211
C	3.76424970528899	1.73941801059579	-0.08510441060812
C	2.02863739148136	-0.03691893643311	-2.95207140794537
C	3.27683882729486	1.49836060406678	-1.50380830293751
C	3.75419822986095	-0.95081275129059	-1.46720173257374
H	-1.58321602685255	3.12539770870335	0.61463289430789
H	-1.26257869204969	2.29909129539846	2.15777694730391
H	-2.77582509135092	3.20654290082566	1.94885947302401
H	-4.66695962986075	1.16536188787675	0.12741143204575
H	-4.02022738405592	2.79345867866299	0.05164967883790
H	-1.57239546694977	-1.02448589723815	-3.01341432227809
H	-1.25607813263679	0.72597284204446	-3.06370522662957
H	-2.76564459829844	0.08884135207299	-3.75177854031314
H	-2.48224372129282	2.20402693723728	-1.76354578259878
H	-4.09280513155680	1.63187366916550	-2.22403180425671
H	1.56186635434981	-2.08766675713905	2.39478184004117
H	1.24259196536249	-3.00989774732327	0.90661264550772
H	2.75033830555338	-3.29070219581253	1.80364597525384
H	2.46366690493367	-2.62917797904695	-1.02602836747811
H	4.07528958158479	-2.75071635090168	-0.30443469176693
H	4.65941558031088	-0.70398325093367	0.95425617390227
H	4.00212944013867	-1.44893240504108	2.39913686138292
H	1.58321979593241	3.12540311295477	0.61462417495573
H	1.26257511139651	2.29909790014643	2.15776713800531
H	2.77582383139576	3.20654734705692	1.94885507363301
H	2.47293155234842	0.42591910342252	2.78996239051322
H	4.08817205371958	1.10235347107760	2.53157356813624
H	4.66696025288212	1.16536288166968	0.12740967507645
H	4.02022793652827	2.79345952035213	0.05164196624900
H	1.57238958534257	-1.02449328098752	-3.01340526414184
H	1.25607836722892	0.72596624742452	-3.06370317760880
H	2.76564110314384	0.08882671168691	-3.75177714437515
H	2.48224609157359	2.20402173424838	-1.76355282135615
H	4.09280718115089	1.63186523135907	-2.22403534269147
H	4.66138411938289	-0.48571174072236	-1.07951618295267
H	4.00412038666826	-1.36131042534033	-2.44919559754505

PBE fully optimized model

Cr	-1.34959726022136	-0.00241540045090	0.00159350210728
Cr	1.34959707362663	-0.00241495962636	0.00159323494332
O	-0.00000010050946	-0.15638310892217	1.48781981598983

O	0.00000004508984	1.35845594113029	-0.61362107614704
O	-0.00000021014605	-1.21981677141294	-0.86688073427499
H	0.00000022403784	0.53561552385173	2.17154439140937
H	0.000000190587447	1.59613086885679	-1.55696085973398
H	-0.000000133941887	-2.15132095960930	-0.58553525424747
N	-2.70524016932110	-1.47031349343035	0.71096108001699
C	-2.05486828729460	-2.54504999990944	1.50774520391590
C	-3.28338174563803	-2.04791714309346	-0.54421579629827
C	-3.76207689894652	-0.79627590969454	1.55256074176901
H	-1.59310029605397	-2.11377416305775	2.40202353122164
H	-1.28038934559168	-3.03931667423510	0.90876828897714
H	-2.79707819407222	-3.30272691427446	1.80138123392941
H	-2.49085225872377	-2.63982318945874	-1.02401181982790
H	-4.11011821765156	-2.73915710284334	-0.31038154702930
H	-4.67821323728999	-0.69817112419575	0.95892296229831
H	-4.01942571854053	-1.43511268350511	2.40899315249634
N	-2.69926703518859	1.35174295578955	0.91747080859573
N	-2.69925963434367	0.11990539930753	-1.62892341247233
C	-3.75847546320576	-0.94475687552015	-1.47179407752803
C	-3.27929355381021	0.55541021357595	2.04563824853083
N	2.70523956147901	-1.47031351760771	0.71096132307233
N	2.69926642340251	1.35174311550754	0.91747160897758
N	2.69926037155770	0.11990615440221	-1.62892286527375
C	-2.04271847733342	2.57657944067327	1.44809691140461
C	-3.75584292650850	1.74785919164366	-0.08592123429056
C	-2.04089889875670	-0.03471572936809	-2.95386542119212
C	-3.27621619280397	1.49638538594101	-1.50361230966558
H	-4.67727448672875	-0.47876165657115	-1.09752440320637
H	-4.00943460881644	-1.36741490712257	-2.45474716681854
H	-2.48558569599563	0.43050898675739	2.79611550005565
H	-4.10201660483972	1.10727362166440	2.52996800763729
C	2.05486730917548	-2.54505016168714	1.50774488494451
C	3.28338150995283	-2.04791687664078	-0.54421546884980
C	3.76207581774391	-0.79627604936754	1.55256159105550
C	2.04271797736664	2.57657964372588	1.44809776421256
C	3.27929220281943	0.55540994637769	2.04563916989555
C	3.75584304058548	1.74785939767591	-0.08591966284726
C	2.04090031396165	-0.03471474354918	-2.95386528230181
C	3.27621723569172	1.49638596554338	-1.50361115198239
C	3.75847589518893	-0.94475639202342	-1.47179311377064
H	-1.58200365938157	3.13363198796407	0.62565215568612
H	-1.26597336272973	2.30250697088451	2.17223954884688
H	-2.78068626248789	3.21268975601747	1.95995841691781
H	-4.67397988908186	1.18880755899492	0.12818064586289
H	-4.00836514533819	2.81007641130964	0.03923657924886
H	-1.57979500160326	-1.02556455491081	-3.02245176380801
H	-1.26374967291114	0.72917726489519	-3.07791497716755
H	-2.77730121603636	0.08989111670974	-3.76215823789941
H	-2.48193821989293	2.20699459849052	-1.77381702160968
H	-4.10035332124477	1.64040237320790	-2.22197549423571
H	1.59309871477052	-2.11377448446859	2.40202297263480
H	1.28038883029362	-3.03931679187677	0.90876736036870
H	2.79707711633584	-3.30272703795949	1.80138127375447

H	2.49085204861455	-2.63982249662707	-1.02401204307399
H	4.11011774629781	-2.73915714140340	-0.31038117665481
H	4.67821245723667	-0.69817113933125	0.95892431311972
H	4.01942422121058	-1.43511294368649	2.40899402375786
H	1.58200409129089	3.13363285376574	0.62565293984496
H	1.26597214137142	2.30250719015921	2.17223962430551
H	2.78068564881178	3.21268934508677	1.95996021961776
H	2.48558385557391	0.43050839789253	2.79611583445093
H	4.10201495722643	1.10727321681792	2.52996962852246
H	4.67397982797954	1.18880766685932	0.12818277979514
H	4.00836524856574	2.81007656793101	0.03923849427929
H	1.57979596860476	-1.02556335497797	-3.02245174659571
H	1.26375152115250	0.72917862260723	-3.07791551550454
H	2.77730311159923	0.08989163065958	-3.76215776176562
H	2.48193970314147	2.20699549290571	-1.77381634761725
H	4.10035493392150	1.64040286943176	-2.22197371250005
H	4.67727471772619	-0.47876139836184	-1.09752269009106
H	4.00943562217967	-1.36741414523383	-2.45474615018926

TPSSh fully optimized model

Cr	-1.35424450239280	0.00748246778796	-0.00087595645706
Cr	1.35423764131845	0.00747803055009	-0.00087750355078
O	-0.00000294430974	-0.13734660180713	1.46342333077295
O	-0.00000064383679	1.35420350893235	-0.59959802230353
O	-0.00000516089286	-1.18217624605433	-0.86562559483160
H	-0.00000065463206	0.52075486357441	2.16950923336362
H	0.00000446473449	1.64878725909317	-1.51878718478551
H	-0.00000926896581	-2.12530440890393	-0.66035454411104
N	-2.68346617865321	-1.45853826988486	0.70650005032200
C	-2.01822727274717	-2.52465540625361	1.50592497177303
C	-3.25911308583331	-2.04955652529081	-0.54278797058362
C	-3.74827281074952	-0.80152247456954	1.54881850901734
H	-1.56748557922213	-2.08271923805020	2.39129571316802
H	-1.24243826043958	-2.99862043316970	0.90648770606852
H	-2.74840997387176	-3.28356694917433	1.79607780436372
H	-2.46291984415168	-2.62337513441757	-1.02093781896581
H	-4.07044743926176	-2.74311239041734	-0.30244269679464
H	-4.65448299937734	-0.70680487372819	0.95372217138132
H	-3.99500774926338	-1.44490669699879	2.39456976728496
N	-2.69755450329625	1.34136962911627	0.91026422821942
N	-2.69230526823111	0.11718842081111	-1.61665366474216
C	-3.74849616889413	-0.94865197019848	-1.46353644818261
C	-3.27063403754831	0.54952804549553	2.04434124343513
N	2.68346715675698	-1.45854069314242	0.70650003406182
N	2.69754925024949	1.34136611134027	0.91026654207433
N	2.69230403104748	0.11718547928447	-1.61665262689138
C	-2.04437616396754	2.57225987860668	1.43663608392829
C	-3.76194284730143	1.73300596201565	-0.08408294061084
C	-2.03228717940052	-0.03618283988186	-2.94309134997238
C	-3.27725483448617	1.49033558111027	-1.50018850579138
H	-4.65645471974087	-0.48734410738601	-1.07991760798513
H	-3.99664215151405	-1.36168809799084	-2.44226987052617
H	-2.47549715669751	0.42734931293811	2.78234874695929

H	-4.08755174458298	1.09782217898898	2.52290059499979
C	2.01823189480386	-2.52466013170271	1.50592432110894
C	3.25911692194754	-2.04955805616288	-0.54278693277931
C	3.74827350165531	-0.80152393465555	1.54881874867098
C	2.04437438874437	2.57225673960399	1.43664047370217
C	3.27063260709400	0.54952529364165	2.04434238389264
C	3.76193758070494	1.73300459398023	-0.08408076294943
C	2.03228955044192	-0.03618719210796	-2.94309210428304
C	3.27724995734855	1.49033424715459	-1.50018655506513
C	3.74849826690828	-0.94865216224951	-1.46353430216360
H	-1.59575047514265	3.12234814848417	0.61291937461478
H	-1.26826445350661	2.29664085726858	2.14911186944439
H	-2.78162146845096	3.19639860592609	1.94666596437982
H	-4.66409353100933	1.16248658840109	0.12799867351868
H	-4.01827672254151	2.78498397644774	0.04889460213876
H	-1.57918667365396	-1.02245710553356	-3.00817218975222
H	-1.25884477264019	0.72228568282228	-3.05436504943444
H	-2.76640836866444	0.09214024180044	-3.74175962042542
H	-2.48702512015610	2.19699107950093	-1.76109217570029
H	-4.09281437247312	1.62358792037224	-2.21722220410103
H	1.56748953447666	-2.08272559171093	2.39129530400812
H	1.24244410784823	-2.99862712397942	0.90648689200259
H	2.74841706997603	-3.28356963121360	1.79607623870542
H	2.46292569126273	-2.62337849835601	-1.02093792725634
H	4.07045302720973	-2.74311163538248	-0.30244048876426
H	4.65448346115229	-0.70680401028077	0.95372228032966
H	3.99501075900995	-1.44490851377397	2.39456915731191
H	1.59574566134859	3.12234477429960	0.61292534612400
H	1.26826627874473	2.29663922181641	2.14912084106002
H	2.78162298309563	3.19639495340303	1.94666639317082
H	2.47549786087627	0.42734489313183	2.78235173581885
H	4.08755032211489	1.09782125435258	2.52289983946985
H	4.66408898713428	1.16248602569396	0.12799994420443
H	4.01827034865908	2.78498276510688	0.04889794787615
H	1.57919077794174	-1.02246221135116	-3.00817477609090
H	1.25884680990156	0.72228058908288	-3.05436842804018
H	2.76641276635084	0.09213636615134	-3.74175868249209
H	2.48701845128170	2.19698799301717	-1.76108932637069
H	4.09280944357511	1.62358920085783	-2.21721985740965
H	4.65645441062758	-0.48734137231740	-1.07991321549768
H	3.99664791915730	-1.36168656486501	-2.44226768508526

TPSS0 fully optimized model

Cr	-1.35461844468457	0.01030134915028	-0.00036785357237
Cr	1.35460627554169	0.01028766894216	-0.00036525364237
O	-0.00000588214374	-0.12970118799346	1.45155120801506
O	0.00000292473005	1.34610798392847	-0.59377291588079
O	-0.00000910910315	-1.16857982968105	-0.85713810783599
H	-0.00000057041420	0.50498071587699	2.16949417834031
H	0.00001659872954	1.66621714198073	-1.49702289002188
H	-0.00001645629844	-2.11078946339894	-0.68259106463514
N	-2.67339911111309	-1.45130156568468	0.70356135855556
C	-2.00851407915116	-2.50817268431647	1.49850885068351

C	-3.24301800991518	-2.03991999715892	-0.53768614986808
C	-3.73218022931389	-0.80082807042842	1.53957397601096
H	-1.56596835729844	-2.06861633902905	2.38512529690937
H	-1.22818762790626	-2.97477350676166	0.90582277996233
H	-2.73173624563119	-3.27082225521605	1.78325561613231
H	-2.44925683633735	-2.61105038331769	-1.01556309312110
H	-4.05049648814284	-2.73325389130283	-0.30007584968826
H	-4.63699543959037	-0.70854451203647	0.94862127442304
H	-3.97786437170656	-1.44096537126814	2.38359526491426
N	-2.69262948322448	1.33541094045243	0.90570000677798
N	-2.68419264461375	0.11604977070504	-1.60887031864223
C	-3.73106111423689	-0.94418670057675	-1.45717943352817
C	-3.25982474988068	0.54760653832998	2.03240140332292
N	2.67340169506338	-1.45131092471342	0.70356296606939
N	2.69262146966224	1.33540352639561	0.90570303616722
N	2.68419091605287	0.11604005386485	-1.60886570503663
C	-2.04395478963474	2.55968070579167	1.42730315944783
C	-3.75004229511303	1.72177047641494	-0.08213637519792
C	-2.02511242854117	-0.03613959409609	-2.92557275274893
C	-3.26727802077698	1.47916015744141	-1.49369740274825
H	-4.63858421436274	-0.48799878784660	-1.07669787406535
H	-3.97795168361674	-1.35807409562146	-2.43195858981660
H	-2.46796620480518	0.42576240019755	2.76910833348445
H	-4.07496081004362	1.09138766082594	2.51090790465842
C	2.00852713933388	-2.50818675959279	1.49851202571683
C	3.24302745747488	-2.03992548380151	-0.53768345032222
C	3.73218126500942	-0.80083134462280	1.53957340287103
C	2.04394808620047	2.55967351228407	1.42730742648811
C	3.25982392903643	0.54760173096091	2.03240217083485
C	3.75003130716960	1.72176835431834	-0.08213518208022
C	2.02511326705153	-0.03615634534787	-2.92556954574355
C	3.26726619674450	1.47915459039843	-1.49369475733122
C	3.73106599610898	-0.94418841585787	-1.45717405276677
H	-1.60454507774423	3.11338826389114	0.60543105991762
H	-1.26301629286947	2.28871837078775	2.13074494534800
H	-2.77665806439953	3.17875265713877	1.94258158926350
H	-4.64965047563973	1.15346736661767	0.12811948042436
H	-4.00857613002237	2.76990491957056	0.04819634547962
H	-1.57850460387564	-1.02146858318047	-2.99401914333719
H	-1.24853484199164	0.71434734816036	-3.03390715032894
H	-2.75310697008017	0.09757757127182	-3.72424510176323
H	-2.48191322916497	2.18667909672878	-1.75316737296165
H	-4.08016938195859	1.61207467832019	-2.20833363365613
H	1.56598182567186	-2.06863346904754	2.38513023464803
H	1.22820268344916	-2.97479441207307	0.90582840411117
H	2.73175582208889	-3.27083070160520	1.78325705566052
H	2.44927166767318	-2.61106100634851	-1.01556303590798
H	4.05051071132762	-2.73325266754748	-0.30007005424726
H	4.63699542518015	-0.70854449964109	0.94861903567285
H	3.97787113512707	-1.44096687841320	2.38359424300208
H	1.60452659456526	3.11337543631119	0.60543812853344
H	1.26301978248557	2.28871297533065	2.13076156116951
H	2.77665567229931	3.17875088320838	1.94257354938842

H	2.46796868236498	0.42575519529286	2.76911207895678
H	4.07496010625791	1.09138675921493	2.51090423116255
H	4.64964385633020	1.15347177868799	0.12811984241322
H	4.00855864293421	2.76990461956547	0.04819617059955
H	1.57850890451370	-1.02148705844792	-2.99401483950417
H	1.24853374368349	0.71432773562272	-3.03390931263666
H	2.75310883311605	0.09756041558786	-3.72424121531210
H	2.48189578965124	2.18666808530993	-1.75316282936649
H	4.08015527136887	1.61207503721940	-2.20833273808893
H	4.63858494875689	-0.48799479366774	-1.07668849335941
H	3.97796292559164	-1.35807124345503	-2.43195358477281

B3LYP fully optimized model

Cr	-1.36570100875668	0.00247211556123	0.00192101894698
Cr	1.36569479694205	0.00247974485658	0.00191134631195
O	0.00000183407565	-0.14883101647043	1.46839158373908
O	-0.00000473592266	1.34851670566811	-0.59967184197994
O	-0.00000315166947	-1.19276647648120	-0.86134243025103
H	0.00000268653727	0.47637523218986	2.19981033443776
H	-0.00000134924858	1.66594674074720	-1.50807096088787
H	-0.00000222395008	-2.13718016849939	-0.67657044177225
N	-2.70746399549712	-1.46790214157633	0.71217438457158
C	-2.04660453816538	-2.53672088197199	1.50590919899499
C	-3.28564800891371	-2.04799613980897	-0.53830468886114
C	-3.76277355366450	-0.79937442693066	1.55477168130510
H	-1.60210131131184	-2.10635604052710	2.39858857243469
H	-1.26470500516673	-3.00685682095156	0.91443446021548
H	-2.77391819717606	-3.30015741870749	1.78763895433906
H	-2.50249232932215	-2.63928879496523	-1.01271834972025
H	-4.10794497682569	-2.72861305754509	-0.30257440375775
H	-4.67428966891541	-0.70952088118804	0.97116765504175
H	-4.00767455069043	-1.43134522786540	2.40790024518619
N	-2.71022883423395	1.35146233266905	0.91562916894816
N	-2.70581002493153	0.11760784209194	-1.62749551408586
C	-3.75824593082792	-0.94969629536078	-1.47199217340516
C	-3.29000055668053	0.55750457046155	2.04171798482405
N	2.70745918889793	-1.46789613096727	0.71217406630528
N	2.71022747948522	1.35146787795217	0.91562142526979
N	2.70581315768724	0.11760735882814	-1.62749935702375
C	-2.05135596044180	2.57424786085057	1.44468090298088
C	-3.76390509196571	1.74549412974274	-0.08723684652666
C	-2.04128901498626	-0.03439438895399	-2.94825133325061
C	-3.28863668474104	1.48857624629612	-1.50492448154973
H	-4.67279516877471	-0.49208473836487	-1.10617389907928
H	-3.99856273929664	-1.37401195157286	-2.44632880285113
H	-2.50725159090900	0.44041204410533	2.79119298598608
H	-4.11227836147857	1.10186678045552	2.51342395598280
C	2.04659695259455	-2.53671207327769	1.50590995967950
C	3.28564544328701	-2.04799444373869	-0.53830106669939
C	3.76276689098016	-0.79936823584245	1.55477293142030
C	2.05135892830628	2.57425712527458	1.44466902989991
C	3.28999495437762	0.55751257865960	2.04171418670316
C	3.76390859463397	1.74549346048356	-0.08724198058952

C	2.04129562692406	-0.03439858768102	-2.94825644825894
C	3.28864357561493	1.48857402602854	-1.50493057937225
C	3.75824753056161	-0.94969739340541	-1.47198935137699
H	-1.60607575742017	3.13146562091590	0.62559807269785
H	-1.27016595258390	2.29884969211481	2.14905682537265
H	-2.78001682512424	3.20009634570872	1.96289234735822
H	-4.67523580756962	1.19437994274474	0.12564046565711
H	-4.00997232496552	2.80010311379160	0.03255411777714
H	-1.59144754267806	-1.02052706863521	-3.01800175124313
H	-1.26275247507359	0.71646406542216	-3.05957521586625
H	-2.76727615378491	0.09759998801177	-3.75243598063875
H	-2.50738977973184	2.19777784083936	-1.77851999815293
H	-4.11050401292764	1.62230349631815	-2.21319850992340
H	1.60208747379931	-2.10634393046398	2.39858459257958
H	1.26470248383573	-3.00685273464629	0.91443219740081
H	2.77390942774827	-3.30014676994408	1.78764823127192
H	2.50249062700280	-2.63928703530858	-1.01271606258381
H	4.10794095427602	-2.72861209757904	-0.30256717962636
H	4.67428543731832	-0.70951769498665	0.97117250018190
H	4.00766416245729	-1.43133662758205	2.40790446070380
H	1.60608442298098	3.13147630419545	0.62558403165295
H	1.27016509148651	2.29886394818164	2.14904260827895
H	2.78002143336990	3.20010298419405	1.96288153092549
H	2.50724469128551	0.44042261939850	2.79118819614804
H	4.11227244413019	1.10187489884446	2.51342048969792
H	4.67523637004156	1.19437607543517	0.12563963991533
H	4.00998018538002	2.80010155949994	0.03254771649676
H	1.59145228835595	-1.02053066518223	-3.01800438080778
H	1.26276114656034	0.71646132454653	-3.05958509276042
H	2.76728605079320	0.09759092206810	-3.75243918792301
H	2.50740011265849	2.19777767885973	-1.77853054069488
H	4.11051386728081	1.62229713888503	-2.21320203101728
H	4.67279510688916	-0.49208582577392	-1.10616691586251
H	3.99857056076768	-1.37401450114227	-2.44632378724095