Supporting Information

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S1. Optimized geometries of all the stationary points including the transition states.

All the values are in hartrees except ZPE which is in kcal mol^{-1} unless stated otherwise.

Name – INT-A2\\G=-1718.870460\\H=-1718.779880\\SCF E(PBE-D3/BS2)=-1719.38517901708\\ZeroPoint=341.290

Angstroms

Atom	x	y	z
Fe1	2.1403736459	12.2760993482	10.4589552677
O2	0.8467199309	13.6796097556	12.6277364729
P3	0.2556187624	12.3970249782	9.2214920995
N4	2.3343937435	10.3639045933	9.3424998271
C5	1.0171936513	9.6909804120	9.2544164785
H6	0.6775263977	9.4715255579	10.2807273609
H7	1.0944546104	8.7299141607	8.7036228824
C8	0.0470059328	10.6414884211	8.5452248961
H9	-0.9965142213	10.3011365607	8.6517851739
H10	0.2714178543	10.6603282205	7.4634323861
P11	3.5424792818	11.2819385702	11.9086602601
C12	0.1401841742	13.4764020152	7.6668516984
H13	0.2392479124	14.5033337227	8.0695962317
C14	1.3588118301	13.2060833276	6.7675097222
H15	1.2695910070	12.2258876638	6.2633715776
H16	2.2947355580	13.2074292035	7.3550439130
H17	1.4193719406	13.9704860590	5.9723212952
C18	-1.1775429434	13.3696902851	6.8834611375
H19	-1.1292980934	14.0098923585	5.9837904442
H20	-2.0537742912	13.6909887242	7.4691176056
H21	-1.3573647018	12.3355634866	6.5393582212
C22	-1.4336833771	12.6657348030	10.0201947474
H23	-2.1558064723	12.3821219435	9.2304305236
C24	-1.6722974292	14.1366608511	10.3979883591
H25	-1.5889926617	14.8115443147	9.5302046938
H26	-0.9546334012	14.4692447490	11.1637454860
H27	-2.6888005031	14.2560093285	10.8140964403
C28	-1.6526536870	11.7297211194	11.2199994812
H29	-1.4811949499	10.6706679118	10.9629188604
H30	-2.6941254809	11.8216508807	11.5781225223
H31	-0.9817092428	11.9893668039	12.0523509451
C32	3.4798727320	9.5119583444	9.7599463204
H33	4.3766302649	9.9421756345	9.2873169383
H34	3.3594188226	8.4809379015	9.3702628094

C35	3.6422547431	9.5114560184	11.2787641466
H36	4.5888017297	9.0267476564	11.5756991811
H37	2.8270250273	8.9422651847	11.7564989496
C38	3.0245426212	10.9821450227	13.7027611169
H39	3.7112488657	10.1904012742	14.0611568340
C40	1.5840202916	10.4535799736	13.8098243501
H41	0.8600053201	11.2200957522	13.4954345766
H42	1.3654372083	10.1842373477	14.8589619990
H43	1.4103629789	9.5549566291	13.1946890437
C44	3.2114391111	12.2329628641	14.5797273526
H45	4.2457313820	12.6122247668	14.5663513755
H46	2.9600206297	11.9931178270	15.6282571243
H47	2.5442149785	13.0449932501	14.2516383659
C48	5.3545772762	11.8099808933	12.0972755828
H49	5.2719049831	12.8584891745	12.4448505992
C50	6.0344576954	11.8208485148	10.7165110039
H51	5.3904202241	12.2982414546	9.9568759591
H52	6.2559975860	10.7898217843	10.3852366390
H53	6.9994598585	12.3556711104	10.7740571554
C54	6.1823775326	11.0089458084	13.1153057998
H55	6.2412460033	9.9416219497	12.8371553384
H56	5.7895634100	11.0695882238	14.1420065879
H57	7.2171666618	11.3958814306	13.1347839879
C58	1.3563150419	13.0479515286	11.7392566274
O59	3.6175904130	12.9428672778	8.9845602780
C60	3.1804015028	13.8565733370	9.8387152541
H61	2.5084737942	14.6560803374	9.4519839566
H62	3.8865776457	14.2219455764	10.6191956127
H63	2.5649055082	10.7387323995	8.4120501970

Name – INT-A3\\G=-1853.768417\\H=-1853.652812 \\SCF E(PBE-D3/BS2)=-1854.36028332021\\ZeroPoint=398.630

Angstroms

Atom	x	y	z
Fe1	2.4399556959	12.2821221141	10.3273903028
O2	2.0005841661	14.6881108424	11.9139014409
P3	0.5249941942	12.5179514471	9.3545664435
N4	2.4864311159	10.4185889876	9.3014417663
C5	1.1998266670	9.9171421623	8.7568484458
H6	0.6515348782	9.4513114309	9.5913838758
H7	1.3878033065	9.1259730076	8.0011639071
C8	0.3963148917	11.0704123526	8.1602680196
H9	-0.6458438192	10.7670509962	7.9571299255
H10	0.8459498897	11.3835931758	7.2017748426
P11	3.2956961582	11.1644048920	12.0108886822
C12	0.0565560329	14.0220689431	8.2612194890

H13	0.2206533215	14.8745788799	8.9488483685
C14	1.0549440569	14.1534833929	7.1041755442
H15	0.8584164620	13.4063445575	6.3147994600
H16	2.0861535004	13.9989941569	7.4590041262
H17	0.9894325870	15.1514889211	6.6338454390
C18	-1.3858023636	14.0770537740	7.7336131217
H19	-1.5097900053	14.9333701937	7.0450386627
H20	-2.1292079653	14.1958619209	8.5372414141
H21	-1.6406199713	13.1635962708	7.1666218646
C22	-1.1064861099	12.3287037766	10.3301080749
H23	-1.9275756208	12.4234786858	9.5965576462
C24	-1.2356247041	13.4479183774	11.3715277109
H25	-1.2577598677	14.4476649521	10.9036109930
H26	-0.3819300149	13.4318737324	12.0685138011
H27	-2.1662651222	13.3296183455	11.9565471805
C28	-1.2003034069	10.9362158056	10.9684527483
H29	-1.4118773030	10.1562031879	10.2174887528
H30	-2.0117030594	10.9020034948	11.7185435830
H31	-0.2537895884	10.6826378635	11.4718000628
C32	3.2709934165	9.3373236978	9.9666330461
H33	4.3295287307	9.5050005646	9.7215426640
H34	2.9892100259	8.3504482332	9.5477221813
C35	3.0729665646	9.3733630918	11.4846461728
H36	3.7692299750	8.6804645081	11.9909671944
H37	2.0468257917	9.0649500554	11.7492849404
C38	2.5855028501	11.1824658686	13.7723513566
H39	3.0605435915	10.3371050826	14.3049678070
C40	1.0688564582	10.9738125629	13.7907309292
H41	0.5655485245	11.7779511516	13.2314221146
H42	0.6949653404	10.9820125444	14.8314434375
H43	0.7700901794	10.0134286414	13.3390064729
H44	3.0653352910	10.8126432055	8.5396925961
C45	2.9437182500	12.4968624720	14.4871554108
H46	4.0314813545	12.6541522982	14.5695756162
H47	2.5300429547	12.4970846490	15.5121310233
H48	2.5162590470	13.3574908184	13.9472205837
C49	5.1673534789	11.2179745905	12.4604662714
H50	5.3143104540	12.2824564239	12.7288791554
C51	6.0271561344	10.9235317864	11.2184389439
H52	5.6332479592	11.4369873061	10.3214546998
H53	6.0552698332	9.8373237690	11.0153393866
H54	7.0731333124	11.2384569889	11.3924643014
C55	5.6217955141	10.3490144237	13.6447992318
H56	5.3879522605	9.2823148289	13.4750679906
H57	5.1648428722	10.6450313905	14.6019647896
H58	6.7184060489	10.4213834161	13.7692399851
C59	2.1928256767	13.6860766921	11.2546781272
O60	4.3008750533	12.3250630203	8.9184318029
C61	4.6200592209	13.4861337619	8.3681895759
H62	5.6985381741	13.6305546573	8.0978426892
H63	3.9987888808	13.8286781928	7.4992301211
N64	4.3596277132	14.6639886965	9.4233088600

C65	5.3932936860	14.6704893266	10.4902271847
C66	4.1362299699	16.0019512916	8.8231571648
H67	6.3404358322	15.0568167243	10.0816164412
H68	5.5132973617	13.6337440544	10.8297102232
H69	5.0556843104	15.3008210636	11.3269654041
H70	5.0380132897	16.3133818440	8.2706524174
H71	3.9204083783	16.7350235117	9.6164734853
H72	3.2813495308	15.9474755115	8.1328940160
H73	3.4643931686	14.2718626461	9.8712139012

Name – INT-A4\\G=-1853.776106\\H=-1853.675247\\SCF E(PBE-D3/BS2)=-1854.37868743330\\ZeroPoint=397.474

Angstroms

Atom	x	y	z
Fe1	2.1045346489	11.9375068563	10.8468703769
O2	-0.1311366802	11.2124832539	12.5358184606
P3	0.8171000639	12.5892325656	9.1365725683
N4	2.3161928626	10.0899127994	9.8649734774
C5	1.2857053373	9.8675852275	8.8149141566
H6	0.3534069529	9.5974138164	9.3369346398
H7	1.5649948226	9.0101649967	8.1691553565
C8	1.0992269225	11.1354581246	7.9806090204
H9	0.2942591304	11.0097698312	7.2357654172
H10	2.0315833885	11.3485302372	7.4354481872
P11	3.6338947747	11.0411154842	12.2302771124
C12	1.2929476433	14.1407015456	8.1210510480
H13	1.9438829397	14.6908791453	8.8194636466
C14	2.1338357731	13.7999298846	6.8797254605
H15	1.5433500915	13.2402208091	6.1321251471
H16	3.0309428735	13.2351212255	7.1639393689
H17	2.4740929142	14.7383215518	6.4075438628
C18	0.1261877298	15.0559721333	7.7114332760
H19	0.5406341741	15.9587851766	7.2279425760
H20	-0.4905781703	15.3941801690	8.5572589484
H21	-0.5376343729	14.5725694876	6.9730774587
C22	-1.0651757833	12.7063015454	9.2973107779
H23	-1.4202718303	13.1463666687	8.3478385921
C24	-1.4351785205	13.6521275771	10.4564409603
H25	-0.8889992646	14.6085369669	10.4200813077
H26	-1.2065850025	13.1835302868	11.4256912526
H27	-2.5160371829	13.8785283167	10.4312176649
C28	-1.7621549432	11.3461071393	9.4673455496
H29	-1.6145221700	10.6852136094	8.5975253626
H30	-2.8507821435	11.5034142819	9.5754293693
H31	-1.4161611546	10.8224765295	10.3727020642
C32	2.3567484701	8.9530857034	10.8305483775
H33	2.6004144468	8.0074888315	10.3063272668
H34	1.3289956744	8.8604645328	11.2181328290
C35	3.3303874038	9.1933286787	12.0007633181

H36	4.2938586393	8.6849118830	11.8320337146
H37	2.9117956672	8.7679625675	12.9277954038
C38	3.6173393851	11.3170984010	14.0915331378
H39	4.3320279604	10.5873916230	14.5155555519
C40	2.2411289354	11.0729928368	14.7250394459
H41	1.5159893427	11.8340386125	14.3997530026
H42	2.3271358242	11.1325781571	15.8247148425
H43	1.8246957363	10.0829236118	14.4756839207
H44	3.2293700657	10.1944961618	9.3963694093
C45	4.1050968631	12.7461872770	14.3884141847
H46	5.1380525219	12.9215381393	14.0460224373
H47	4.0737689444	12.9418973776	15.4749818898
H48	3.4524781618	13.4822720294	13.8868101770
C49	5.4901562542	11.1445719534	11.8365746605
H50	5.7110348120	12.2267572750	11.8648976681
C51	5.7531858469	10.6565354812	10.4016821142
H52	5.0943804657	11.1950254589	9.7003988773
H53	5.5943906113	9.5667892867	10.3045111853
H54	6.8037997634	10.8536495794	10.1241488544
C55	6.3985382913	10.4229914014	12.8454914984
H56	6.1419864311	9.3525875843	12.9407761711
H57	6.3675742279	10.8705853471	13.8514710658
H58	7.4452986341	10.4752265512	12.4952612508
C59	0.8046672943	11.4904869285	11.8483691596
O60	3.4842866304	12.6007866056	9.5418752397
C61	4.1194341808	13.7840802063	9.8709101766
H62	4.8933977671	13.6343630996	10.6846370233
H63	3.4158182615	14.5530498569	10.2671766764
N64	4.7760109110	14.4045695695	8.6974488827
C65	5.8046444037	13.5401033322	8.1337563784
C66	5.3277594594	15.7040094324	9.0551372518
H67	2.0681922971	13.2865513065	11.5269607540
H68	4.5282140704	16.3591740705	9.4438350875
H69	5.7661873630	16.1892115632	8.1652944560
H70	6.1288492129	15.6491881709	9.8362435763
H71	6.2270035828	13.9980406765	7.2218443616
H72	5.3562086968	12.5710575185	7.8662356048
H73	6.6492195456	13.3417402321	8.8419994339

Name-catalyst\\G=-1604.497614\\H=-1604.408226\\SCF E(PBE-D3/BS2)=-1604.97007231294\\ZeroPoint=317.315

Angstroms

Atom	x	y	z
Fe1	1.8707542149	12.0365546566	10.7078885547
O2	2.5805932185	14.8183102890	11.1510032995
P3	0.2822708630	12.4176604549	9.2515126854
N4	2.1031998292	10.4278421461	9.8224022719
C5	1.3370658434	9.9609333203	8.6509234082

H6	0.6348340945	9.1586646760	8.9691112134
H7	2.0252192648	9.4804660593	7.9217363036
C8	0.5669436633	11.0961168474	7.9682916481
H9	-0.3723626348	10.7459107727	7.5064233555
H10	1.1806616403	11.5512450913	7.1726884836
P11	3.3360302358	11.2841145640	12.1359623073
C12	0.2212215138	14.0310754660	8.2818917930
H13	0.0417186761	14.7981898835	9.0591509154
C14	1.5909557808	14.3194566359	7.6435777144
H15	1.8075366731	13.6180474817	6.8187422356
H16	2.4050890354	14.2379036695	8.3806159631
H17	1.6032031657	15.3390356341	7.2197391866
C18	-0.9087022755	14.0927927766	7.2417495319
H19	-0.8712781831	15.0532260890	6.6972741664
H20	-1.9082511764	14.0112200361	7.6985491317
H21	-0.8081301473	13.2861251322	6.4942648951
C22	-1.4881605738	12.1528008460	9.8299528703
H23	-2.1303888600	12.1723333592	8.9286785251
C24	-1.9111044654	13.2759490299	10.7885381532
H25	-1.9068820108	14.2662035459	10.3027356536
H26	-1.2250209438	13.3167340478	11.6527740626
H27	-2.9324980231	13.0922759973	11.1667204631
C28	-1.6036442018	10.7738702386	10.4996029015
H29	-1.4097911216	9.9518520704	9.7907963337
H30	-2.6198588173	10.6306181607	10.9087460808
H31	-0.8744639286	10.6916462460	11.3239549337
C32	3.0122107066	9.3368013293	10.2318535142
H33	3.8800102014	9.3097998764	9.5379142919
H34	2.5029517093	8.3560283593	10.1129679931
C35	3.4929871793	9.4851644880	11.6808512489
H36	4.5178392079	9.1019562204	11.8254017505
H37	2.8325098034	8.9225913125	12.3612805729
C38	2.9810203895	11.3061261881	13.9819437006
H39	3.7916636540	10.7342934885	14.4734212027
C40	1.6338419814	10.6314473454	14.2853800770
H41	0.8213697787	11.1431606750	13.7418580060
H42	1.4211302918	10.6828760047	15.3680932670
H43	1.6160999232	9.5686080693	13.9923339645
H44	0.8899058649	12.2255410450	11.8133816550
C45	2.9916894026	12.7580232157	14.4902228827
H46	3.9722538671	13.2446976741	14.3577465159
H47	2.7448516075	12.7885252775	15.5661012572
H48	2.2390214492	13.3571329010	13.9492392379
C49	5.0736101616	11.9959656465	11.9772911672
H50	4.9356721237	13.0736245665	12.1868353396
C51	5.5307147130	11.8547045497	10.5147556026
H52	4.7555031545	12.2285014879	9.8246585871
H53	5.7334523332	10.7997191943	10.2593822608
H54	6.4628134276	12.4219472595	10.3456737068
C55	6.1039542613	11.4197514084	12.9586489560
H56	6.2195787167	10.3290625322	12.8296564704
H57	5.8366575873	11.6102797219	14.0107005296

H58	7.0938881432	11.8766626049	12.7800650255
C59	2.2708722246	13.6782963363	10.9772332595

Name – TS-A2\\G=-1853.758140\\H=-1853.643561\\SCF E(PBE-D3/BS2)=-1854.34703331495\\ZeroPoint=396.354

Angstroms

Atom	x	y	z
Fe1	2.3675425722	12.2160938578	10.2109527267
O2	2.1722381355	14.8345596683	11.4470352414
P3	0.3544514901	12.3502241327	9.4000358420
N4	2.4026518941	10.3038087609	9.2575199660
C5	1.0598686934	9.7336525156	8.9543196761
H6	0.6393426699	9.3718810597	9.9065034351
H7	1.1626541295	8.8599091177	8.2774933279
C8	0.1623228050	10.8065680361	8.3452074435
H9	-0.8821854273	10.4574455298	8.2713772252
H10	0.5034917493	11.0468936043	7.3220791715
P11	3.3559146845	11.2046679138	11.8757537209
C12	-0.1191026658	13.7467953091	8.1871087711
H13	-0.0572529271	14.6551123233	8.8177111004
C14	0.9696830563	13.8536038512	7.1111184544
H15	0.9156726329	13.0150839391	6.3935354721
H16	1.9628302826	13.8280122612	7.5814533847
H17	0.8681277691	14.7900151189	6.5335155274
C18	-1.5169278088	13.6676523912	7.5552780797
H19	-1.6499674733	14.4792655476	6.8160153509
H20	-2.3266682657	13.7666139643	8.2955154576
H21	-1.6608490923	12.7119421054	7.0200557645
C22	-1.2178075177	12.2983799735	10.4715600805
H23	-2.0791770500	12.3937407466	9.7852215736
C24	-1.2152434590	13.4851661319	11.4448963820
H25	-1.2194922858	14.4540013527	10.9161382339
H26	-0.3132140765	13.4612080048	12.0794868415
H27	-2.1045915646	13.4556788829	12.1003752736
C28	-1.3378183729	10.9534340415	11.2016186550
H29	-1.5791880318	10.1304788276	10.5076171697
H30	-2.1403252640	10.9919793278	11.9608354535
H31	-0.3937331671	10.7048929367	11.7112119887
C32	3.2867123996	9.2938296729	9.9142526548
H33	4.3178963675	9.5147798469	9.6017511099
H34	3.0421312241	8.2756057354	9.5490438195
C35	3.1676802289	9.3854682077	11.4379866277
H36	3.9186152808	8.7393932548	11.9269916374

H37	2.1727124252	9.0467946310	11.7739188801
C38	2.7573709464	11.3036579102	13.6756279034
H39	3.2817045898	10.5057121937	14.2337155365
C40	1.2497133310	11.0685028040	13.7897618120
H41	0.7054031971	11.8283877023	13.2073952956
H42	0.9281269729	11.1338316802	14.8457351197
H43	0.9496418020	10.0769637692	13.4110164561
H44	2.8364510814	10.5668898073	8.3612852289
C45	3.1259978658	12.6714461893	14.2765920961
H46	4.2150491561	12.8352868076	14.3248254114
H47	2.7329917818	12.7570642057	15.3059232381
H48	2.6872710970	13.4870455533	13.6769042813
C49	5.2511652145	11.3136779712	12.2234801448
H50	5.3822563424	12.3775810509	12.4925156332
C51	6.0657815108	11.0671340312	10.9433909002
H52	5.6270796118	11.5964869408	10.0826595638
H53	6.1147145040	9.9886454260	10.7061344704
H54	7.1083066093	11.4096617398	11.0810410369
C55	5.7920793292	10.4576965932	13.3806873156
H56	5.5873725397	9.3831569512	13.2240750587
H57	5.3732123775	10.7406490927	14.3594116272
H58	6.8906883656	10.5674205295	13.4515581150
C59	2.2440281931	13.7285177867	10.9592365539
O60	4.0293763459	12.5438678269	8.8521769845
C61	4.4216754346	13.6370933018	8.3817555587
H62	5.4849746086	13.7769192507	8.0994498746
H63	3.7186200307	14.4400951630	8.0928196199
N64	4.9126232800	15.4361201377	10.0498135158
C65	5.7014670448	14.9681680608	11.1808389073
C66	5.5034125897	16.5509431447	9.3223789854
H67	3.9587644202	15.6478664835	10.3608473082
H68	4.8271125861	16.8673627139	8.5102832486
H69	6.4580136698	16.2309829077	8.8654045378
H70	5.7181058620	17.4376684279	9.9593511819
H71	6.6350209975	14.4987568236	10.8215742846
H72	5.1187709911	14.2076196019	11.7192609408
H73	5.9788613624	15.7750389995	11.8954377201

Name – INT-B1\\G=-1720.058589\\H=-1719.960668\\SCF E(PBE-D3/BS2)=-1720.58781815268\\ZeroPoint=350.043

Angstroms

Atom	x	y	z
Fe1	2.4752309377	11.9824976122	10.5042705156
O2	3.2982520884	14.7224575096	11.0413122669
P3	0.8179505238	12.5207749615	9.1521475282
N4	2.2332124162	10.1908084873	9.8589520149
C5	1.0441773820	9.8052407273	9.0654461853
H6	0.2198735308	9.5037711744	9.7442751903

H7	1.2770498753	8.9113933557	8.4467759313
C8	0.5999003834	10.9590325432	8.1632664037
H9	-0.4236126371	10.8228270432	7.7745627452
H10	1.2914118032	11.0392798548	7.3057554614
P11	3.7197040256	11.0793307123	12.0815010782
C12	0.9385012893	13.9093634253	7.8800015954
H13	0.8117629962	14.8308283921	8.4802484877
C14	2.3356528124	13.9466334262	7.2439135729
H15	2.5288643961	13.0405782650	6.6435975961
H16	3.1234777080	14.0217218970	8.0088969234
H17	2.4222720269	14.8159564439	6.5683186994
C18	-0.1622720043	13.8567366028	6.8066402814
H19	-0.0721620938	14.7278352456	6.1330544516
H20	-1.1782320251	13.8756936796	7.2333576697
H21	-0.0697142222	12.9486760914	6.1858115302
C22	-0.8424743542	12.8770034512	9.9700450386
H23	-1.5463514547	13.1225983122	9.1524823601
C24	-0.7153911117	14.0904934372	10.9057405756
H25	-0.3654571277	14.9954415635	10.3809120831
H26	0.0008833486	13.8731575329	11.7166638823
H27	-1.6949443920	14.3246212720	11.3594630198
C28	-1.3791628126	11.6511287915	10.7243934321
H29	-1.6155628077	10.8146291391	10.0469769174
H30	-2.3070829157	11.9155005470	11.2626074264
H31	-0.6428735625	11.2993299119	11.4676158622
C32	2.6803651173	9.0123802909	10.6354298087
H33	2.8908975818	8.1662168379	9.9458726207
H34	1.8624358144	8.6683603193	11.3019098249
C35	3.9309534701	9.3383296068	11.4564005188
H36	4.8169585673	9.3538082140	10.7967116302
H37	4.1114257030	8.6013253086	12.2576385506
C38	2.9292385677	10.9494705337	13.7878225424
H39	3.6806314625	10.4715359873	14.4442659843
C40	1.6711970391	10.0685344902	13.7648838342
H41	0.9478025339	10.4432888337	13.0203258819
H42	1.1810485414	10.0845650876	14.7548440690
H43	1.9026464201	9.0180799901	13.5259098485
H44	3.3495528046	10.1388621858	8.6139544788
C45	2.6130292681	12.3542498821	14.3270769066
H46	3.5087837973	12.9940858741	14.3931260102
H47	2.1776013454	12.2826728427	15.3395609158
H48	1.8850907159	12.8603924459	13.6701744596
C49	5.4579176844	11.6849223680	12.4967607432
H50	5.2806085191	12.6084139861	13.0811666406
C51	6.2263849553	12.0698126269	11.2241221332
H52	5.6535739307	12.7777459698	10.6052188678
H53	6.4512279162	11.1816618551	10.6077360125
H54	7.1904271659	12.5384632985	11.4901157070
C55	6.2655336745	10.6987851423	13.3584718413
H56	6.4595099138	9.7587099265	12.8129600193
H57	5.7631515371	10.4458803515	14.3061247966
H58	7.2458025148	11.1396249204	13.6135911620

C59	2.9698805537	13.6014891029	10.8120342675
H60	1.4793433795	12.1473631254	11.5685061416
O61	4.0244293030	10.1500976353	7.8453340197
C62	4.6851208936	11.3865134748	8.0202694499
H63	4.7122249685	11.9702049433	7.0799490207
H64	5.7273547163	11.2686443550	8.3811476570
H65	4.1455769227	12.0184297321	8.7781021058

Name – INT-B2\\G=-1720.050232\\H=-1719.956181\\SCF E(PBE-D3/BS2)=-1720.58225792327\\ZeroPoint=349.133

Angstroms

Atom	x	y	z
Fe1	2.5393037557	11.9843131713	10.4418201627
O2	3.1318381355	14.7131540966	11.2304505149
P3	0.8435756395	12.5154382881	9.1252033282
N4	2.2666595836	10.0867584084	9.7569620805
C5	0.9478762106	9.7810663451	9.1384649761
H6	0.2030080723	9.6387396221	9.9401678921
H7	1.0128650134	8.8286771253	8.5729979372
C8	0.5454951077	10.9231428246	8.2042870016
H9	-0.4862549975	10.8137369073	7.8299054786
H10	1.2364469718	10.9368501723	7.3420378001
P11	3.7553100845	11.0623248793	12.0346633723
C12	0.9286463525	13.8512155541	7.7927797901
H13	0.7384586131	14.7892763493	8.3496353976
C14	2.3345648036	13.9313568433	7.1826851794
H15	2.5837476417	13.0072509364	6.6326324245
H16	3.0992491708	14.0787229034	7.9608084083
H17	2.3940269304	14.7713689539	6.4680469647
C18	-0.1464607439	13.6960797111	6.7029044590
H19	-0.1071913383	14.5574609016	6.0123711505
H20	-1.1694103385	13.6474742370	7.1110713035
H21	0.0247373733	12.7855731876	6.1033206252
C22	-0.7792614099	12.9667256262	9.9763651387
H23	-1.4635466600	13.2896062569	9.1688284575
C24	-0.5496091199	14.1434121373	10.9391418523
H25	-0.0989943867	15.0190079363	10.4424339458
H26	0.1247390245	13.8370456719	11.7563936186
H27	-1.5089600560	14.4661121636	11.3812684539
C28	-1.4201353576	11.7788975208	10.7082980475
H29	-1.7032808806	10.9647048427	10.0213632917
H30	-2.3383269894	12.1087374665	11.2268584741
H31	-0.7309104561	11.3722879810	11.4691570461
C32	2.6841633966	8.9595137977	10.6373774875
H33	2.8516743226	8.0539115436	10.0195277296

H34	1.8584612544	8.7314251948	11.3327307989
C35	3.9564161548	9.3160661883	11.4112316021
H36	4.8227041670	9.3284127068	10.7251095658
H37	4.1670153433	8.5846406759	12.2105971093
C38	2.9527406105	10.9453746463	13.7410734639
H39	3.7345090390	10.5502146278	14.4173830977
C40	1.7535380141	9.9872464466	13.7741580740
H41	0.9921996161	10.2888597630	13.0335006332
H42	1.2811894838	10.0112687171	14.7725934727
H43	2.0452426912	8.9435185710	13.5726817074
H44	2.9957803863	10.0802301422	8.8872482141
C45	2.5428480053	12.3494155332	14.2171759051
H46	3.3845134249	13.0627521176	14.2212371579
H47	2.1431308798	12.2984648279	15.2456525057
H48	1.7588855373	12.7584313810	13.5573446821
C49	5.4855386879	11.6467632868	12.5229595550
H50	5.2772389491	12.4787354368	13.2235258261
C51	6.2656354612	12.2190415193	11.3308691168
H52	5.6674871169	12.9558053090	10.7719070877
H53	6.5665823140	11.4213338980	10.6303815090
H54	7.1883372913	12.7125905847	11.6837384040
C55	6.3056002842	10.5737540826	13.2616871175
H56	6.5590361206	9.7348477642	12.5904066639
H57	5.7816844519	10.1599598848	14.1391639969
H58	7.2557311169	11.0085846933	13.6203111255
C59	2.8897965478	13.5971516059	10.9023231482
H60	1.4559684843	11.8734787072	11.4488245916
O61	3.9156113916	10.2633112363	7.8261300539
C62	4.4766382145	11.3971477066	8.2813983339
H63	4.5739160992	12.2308343674	7.5456665948
H64	5.4507970690	11.2893465131	8.8189391424
H65	3.8084383077	11.9646633613	9.1189749812

Name – INT-B3\\G=-1720.034790\\H=-1719.933573\\SCF E(PBE-D3/BS2)=-1720.55430384788\\ZeroPoint=347.603

Angstroms

Atom	x	y	z
Fe1	2.3703263070	12.0641503215	10.6137698343
O2	2.7144912083	14.7553403227	11.6110524478
P3	0.7976381004	12.5687503931	9.1912082580
N4	2.3210385624	10.1457373350	9.7032400075
C5	1.0423849443	9.8443146211	9.0073671735
H6	0.2895167273	9.6551530281	9.7906325644
H7	1.1419992111	8.9205218693	8.4008469920
C8	0.6201679162	11.0289405974	8.1406383569
H9	-0.4002724904	10.8932071511	7.7427727744
H10	1.3026183921	11.1332591648	7.2780931168

P11	3.6999883983	11.1301371422	12.0651665560
C12	0.9974440088	13.9543914323	7.9142750808
H13	0.8765889975	14.8799705831	8.5097854482
C14	2.4167435536	13.9509822419	7.3291832392
H15	2.5884965633	13.0528093617	6.7079616836
H16	3.1695622306	13.9494906489	8.1320004189
H17	2.5677351731	14.8331474161	6.6815955155
C18	-0.0589269813	13.9405025414	6.7963089832
H19	0.0972745780	14.7962031412	6.1153399907
H20	-1.0891543945	14.0107351190	7.1784792950
H21	0.0150696351	13.0217321571	6.1895244194
C22	-0.9394571145	12.9178278377	9.8531819847
H23	-1.5570665340	13.2340571987	8.9919263124
C24	-0.8634067044	14.0615999558	10.8767640661
H25	-0.4364116618	14.9844790088	10.4488270689
H26	-0.2269267178	13.7555347577	11.7243651968
H27	-1.8709907197	14.3034612715	11.2601605170
C28	-1.5798140505	11.6723873877	10.4814647460
H29	-1.7594116639	10.8732377625	9.7425871142
H30	-2.5555238556	11.9336749993	10.9293670026
H31	-0.9267215724	11.2739343010	11.2777119011
C32	2.6852412349	9.0325199694	10.6194686738
H33	2.8286759287	8.0932211121	10.0463909953
H34	1.8297579743	8.8863603056	11.2999306162
C35	3.9393376592	9.3906052861	11.4141435061
H36	4.8221226689	9.4026001351	10.7497939021
H37	4.1340334365	8.6537592974	12.2123246613
C38	3.0879278950	10.9156941416	13.8418903390
H39	3.9333100673	10.5138767829	14.4308527347
C40	1.9161153536	9.9286270297	13.9334312998
H41	1.0975657952	10.2531432776	13.2671184771
H42	1.5297499269	9.8947211676	14.9681038307
H43	2.2079854887	8.9015837384	13.6563646102
H44	3.0605597177	10.2184847558	8.9829729946
C45	2.6822445541	12.2893495766	14.3987837900
H46	3.5119275525	13.0161809231	14.3785321313
H47	2.3426903295	12.1955115773	15.4460256323
H48	1.8561399339	12.7015696474	13.7948669432
C49	5.4702925819	11.7419438256	12.3498187853
H50	5.3367606641	12.6663578058	12.9441531477
C51	6.1316075235	12.1259402825	11.0188066598
H52	5.4929751076	12.8200229774	10.4514822285
H53	6.2993928049	11.2351298168	10.3860934364
H54	7.1165815698	12.5925700240	11.1996783420
C55	6.3552629771	10.7646162662	13.1419558730
H56	6.5025802566	9.8228854940	12.5868558180
H57	5.9393091690	10.5124099999	14.1291707969
H58	7.3535703877	11.2061138544	13.3098409380
C59	2.5474189599	13.6392163859	11.2218912861
H60	1.2091211204	11.5692192858	11.5371473308
O61	4.4004481705	10.2014375278	7.4702237296
C62	5.0098669365	11.2655181393	7.4013350973

H63	5.7570190601	11.4515261066	6.5919134608
H64	4.8281125613	12.0788916685	8.1463055540
H65	3.5170827461	12.3855328082	9.6271077341

Name – TS-B1\\G=-1720.033998\\H=-1719.940682\\SCF E(PBE-D3/BS2)=-1720.56137194968\\ZeroPoint=348.079

Angstroms

Atom	x	y	z
Fe1	2.4461259964	11.9125515354	10.4943575351
O2	2.9517416211	14.6573754852	11.2494136057
P3	0.8126071731	12.3972569683	9.1268278286
N4	2.2569866109	9.9490028970	9.7729954721
C5	0.9984464657	9.6602619925	9.0259529505
H6	0.2095454560	9.4880779762	9.7756905145
H7	1.1121424489	8.7257736234	8.4403385412
C8	0.6194236869	10.8331077540	8.1199146539
H9	-0.3944811158	10.7034942810	7.7029327835
H10	1.3206981392	10.9072000764	7.2685942109
P11	3.6982646639	11.0238045022	12.0605974478
C12	0.9123092332	13.7932350187	7.8530568663
H13	0.6811990650	14.6942727048	8.4539788601
C14	2.3306678942	13.9530459059	7.2900050839
H15	2.5767850756	13.1259408334	6.6003370720
H16	3.0813388808	13.9577925862	8.0953290078
H17	2.4092617285	14.8923601937	6.7144076123
C18	-0.1220552112	13.6778495727	6.7203454551
H19	-0.0704701495	14.5694471500	6.0700005526
H20	-1.1578862918	13.5993226161	7.0885526834
H21	0.0800449516	12.7966083254	6.0868806489
C22	-0.8870353054	12.7534315611	9.8765394142
H23	-1.5333666720	13.0958104718	9.0464170475
C24	-0.7514333462	13.8818235526	10.9120063353
H25	-0.3220295038	14.8034030995	10.4835226741
H26	-0.0919073605	13.5526362197	11.7330262302
H27	-1.7410516786	14.1368209609	11.3317728430
C28	-1.5268760628	11.5118032217	10.5122089902
H29	-1.7509262624	10.7263029043	9.7711924801
H30	-2.4800720270	11.7859477034	10.9989289470
H31	-0.8583862938	11.0903245827	11.2834692529
C32	2.5042526366	8.8997968637	10.8021769803
H33	2.5708610602	7.9026354564	10.3209288227
H34	1.6352157148	8.8930852181	11.4802512728
C35	3.7885798048	9.2252204276	11.5626385254
H36	4.6542422550	9.1290051329	10.8831844595
H37	3.9429332317	8.5411712827	12.4141284550

C38	3.0368185883	11.0420446802	13.8312868335
H39	3.8600578369	10.6788227041	14.4754030099
C40	1.8250774520	10.1193366267	14.0194461473
H41	1.0135556261	10.4112963583	13.3299356275
H42	1.4434924022	10.2030033595	15.0529308372
H43	2.0702433902	9.0586004989	13.8430798955
C44	2.6850756103	12.4853344512	14.2261088067
H45	3.5385241876	13.1759775327	14.1169056913
H46	2.3536403487	12.5247466748	15.2792567685
H47	1.8677458707	12.8559330954	13.5846752682
C48	5.5021154882	11.5081268681	12.3659749988
H49	5.4254865549	12.4152508357	12.9965979686
C50	6.2036307288	11.8910783393	11.0564197830
H51	5.6568412209	12.6919946845	10.5363603872
H52	6.2610355854	11.0275835365	10.3704048417
H53	7.2343825595	12.2317251101	11.2604883874
C54	6.3025304635	10.4403040038	13.1321804742
H55	6.4426584966	9.5334205509	12.5187452085
H56	5.8234852496	10.1371978098	14.0777285640
H57	7.3070952949	10.8269930338	13.3803705234
C58	2.7239592299	13.5243111547	10.9628796760
H59	1.3130868100	11.6077777505	11.4921157739
O60	4.7230832500	9.9417963416	8.3049762587
C61	4.6320577903	11.1565806740	8.0306709852
H62	3.0480182037	9.8721753349	9.1018385650
H63	3.6296388738	12.1372362208	9.4566742623
H64	3.8438949210	11.5431973640	7.3488198608
H65	5.4422943319	11.8773727396	8.2758932263

Name – INT-B5\\G=-1853.796418\\H=-1853.691016\\SCF E(PBE-D3/BS2)=-1854.39626901779\\ZeroPoint=395.399

Angstroms

Atom	x	y	z
Fe1	1.9042939059	12.2798840868	10.8523861496
O2	1.6282680169	14.8564781955	12.1762051324
P3	0.1514946426	12.5460963818	9.5483054412
N4	2.3960720571	10.8791086961	9.6671240627
C5	1.4421253240	10.3016214904	8.6885962642
H6	0.8643609606	9.4865321004	9.1725764152
H7	2.0007001150	9.8289705782	7.8516453752
C8	0.4979489766	11.3769283984	8.1409599314
H9	-0.4182348448	10.9481313716	7.7009355761
H10	1.0142944320	11.9632496975	7.3624266166
P11	3.4447168449	11.4822420023	12.2034242230
C12	-0.2064699838	14.2124654472	8.7468855087
H13	-0.6092824801	14.8272782073	9.5745971132

C14	1.1071573932	14.8540516880	8.2732582768
H15	1.5819005804	14.2584690956	7.4748207862
H16	1.8291946376	14.9323613198	9.1018769979
H17	0.9163195111	15.8665888241	7.8762925176
C18	-1.2450612142	14.1489229862	7.6154928183
H19	-1.4319422636	15.1627211613	7.2184065539
H20	-2.2134587314	13.7418770639	7.9490069660
H21	-0.8838599261	13.5284742753	6.7768159421
C22	-1.5190281202	12.0280657805	10.2423586971
H23	-2.2584419247	12.1991346079	9.4368193511
C24	-1.8822570289	12.8951391436	11.4586034607
H25	-1.9348372713	13.9685117190	11.2115890835
H26	-1.1308185630	12.7674605706	12.2569751118
H27	-2.8670775500	12.5950461304	11.8587432618
C28	-1.5240289591	10.5350569840	10.6056191529
H29	-1.3796165219	9.8886321051	9.7246073648
H30	-2.4907759670	10.2608611440	11.0644046986
H31	-0.7246766581	10.3120539859	11.3331939300
C32	3.3818589418	9.8330997471	10.0205500106
H33	3.9283848809	9.5118405838	9.1071773358
H34	2.8499741399	8.9304515977	10.3887776369
C35	4.3728963122	10.3214822223	11.0812907757
H36	5.1675225191	10.9261180084	10.6116546609
H37	4.8558549534	9.4858700442	11.6164994579
C38	2.8222142404	10.4354893874	13.6427161107
H39	3.7196537654	10.0953447536	14.1937376381
C40	2.0569274899	9.2013804664	13.1411557633
H41	1.2390545501	9.5016879518	12.4636195118
H42	1.6131852605	8.6580707243	13.9945350749
H43	2.7112205331	8.4962898373	12.6035144600
H44	0.9437592292	11.7722473654	11.8385880220
C45	1.9504947149	11.2849165825	14.5820986472
H46	2.4870597741	12.1614618003	14.9823225462
H47	1.6155425175	10.6769786164	15.4411654559
H48	1.0582880641	11.6521394104	14.0466356093
C49	4.7640552458	12.5473034446	13.0328575311
H50	4.2308023168	13.0021179185	13.8899352126
C51	5.2297140704	13.6811544694	12.1080485774
H52	4.3829257343	14.2769837236	11.7347962855
H53	5.7745470612	13.2862923267	11.2337084553
H54	5.9192636985	14.3541482832	12.6481738718
C55	5.9576135751	11.7377813860	13.5689633031
H56	6.5321666793	11.2815369769	12.7439076329
H57	5.6550603265	10.9327660146	14.2586441764
H58	6.6458988619	12.4032087045	14.1203462277
C59	1.7459273570	13.8036239352	11.6319760363
O60	3.5719870286	12.3533783829	7.6243298554
C61	4.2923516975	13.4373486243	8.1652927731
H62	3.1828869853	11.8640491889	8.4199187181
N63	5.6984322586	13.3871483396	7.7519741887
C64	6.3908982383	12.2066906349	8.2591698357
C65	6.4016170769	14.6186832969	8.1007661067

H66	4.1574187893	13.4354924113	9.2850622674
H67	3.8910948771	14.4013795288	7.7917312228
H68	5.8655444263	15.4894417968	7.6857107267
H69	7.4185846049	14.6062657406	7.6723507098
H70	6.5029553460	14.7757061049	9.2016213983
H71	7.3732381339	12.0983164778	7.7682640392
H72	5.7874655780	11.3144269513	8.0313136462
H73	6.5673984601	12.2413775204	9.3617349472

Name – INT-B6\\G=-1853.788387\\H=-1853.685443\\SCF E(PBE-D3/BS2)=-1854.39162675521\\ZeroPoint=396.068

Angstroms

Atom	x	y	z
Fe1	2.1442103242	12.4010415993	10.6712552727
O2	1.8867649656	14.9062159704	12.1107876322
P3	0.2778632917	12.6160396247	9.4844658753
N4	2.4948961132	10.7370825836	9.4996257264
C5	1.2891341249	10.1420309041	8.8585964946
H6	0.7209979064	9.5924499550	9.6282950669
H7	1.5994295502	9.4105019525	8.0844067324
C8	0.4402763046	11.2474001909	8.2276315889
H9	-0.5294535079	10.8669065714	7.8653282574
H10	0.9969013549	11.6807358391	7.3782978870
P11	3.5232909922	11.4480398284	12.1026758250
C12	-0.2889696325	14.1394473181	8.5098303238
H13	-0.8069221630	14.7463446255	9.2771888625
C14	0.8861398681	14.9616036497	7.9704101476
H15	1.4171183863	14.4124043991	7.1746034072
H16	1.6097055498	15.1951588333	8.7683776511
H17	0.5245495761	15.9111240788	7.5374418426
C18	-1.2860331137	13.8032878899	7.3867138034
H19	-1.6781940150	14.7357169170	6.9426413541
H20	-2.1513908549	13.2161266982	7.7361121795
H21	-0.7944800943	13.2347729559	6.5785407592
C22	-1.3325309734	12.2751350419	10.4210649540
H23	-2.1428394699	12.5306501396	9.7120460814
C24	-1.4331638753	13.2008485141	11.6444356213
H25	-1.3434094990	14.2685550472	11.3816686401
H26	-0.6310531164	12.9653859066	12.3635628978
H27	-2.4059255385	13.0610465242	12.1485566164
C28	-1.5037951984	10.8075221388	10.8343533903
H29	-1.5211255780	10.1237214817	9.9699093244
H30	-2.4570022902	10.6792361039	11.3781674005
H31	-0.6883915414	10.4957614378	11.5094791684
C32	3.3696769547	9.6459878933	10.0249608776
H33	3.8971663570	9.1651825956	9.1773430705
H34	2.7225979653	8.8779281634	10.4802987856
C35	4.3765367735	10.1565624416	11.0609770500

H36	5.2150257920	10.6722470469	10.5639090327
H37	4.7958859494	9.3249756530	11.6535920314
C38	2.7106184648	10.5022232215	13.5315198196
H39	3.5425266039	10.1779359475	14.1850526335
C40	1.9439911253	9.2533841814	13.0752747068
H41	1.1893520908	9.5129342158	12.3131815082
H42	1.4149653692	8.8002625686	13.9328731908
H43	2.6120176753	8.4826900495	12.6570224820
H44	1.1663845129	11.6778203890	11.5297921679
C45	1.7927330581	11.4448469848	14.3271246401
H46	2.3179157193	12.3414637184	14.6977265382
H47	1.3743651928	10.9176733655	15.2030738512
H48	0.9578585282	11.7845626891	13.6912811173
C49	4.8889412519	12.3071017407	13.0966900577
H50	4.3448854724	12.6866956581	13.9828306809
C51	5.4828039358	13.5136987626	12.3630899088
H52	4.6970575661	14.1992287332	12.0107548045
H53	6.0698399967	13.1964150324	11.4859526131
H54	6.1622611905	14.0711587580	13.0323424241
C55	5.9958038849	11.3465062424	13.5668517228
H56	6.5825596088	10.9694037881	12.7113026013
H57	5.6062602049	10.4749596116	14.1186774463
H58	6.6940401030	11.8770343573	14.2388004827
C59	1.9868422808	13.8793363934	11.5189971127
O60	3.5760209416	12.0230158517	7.5438785247
C61	3.8410688544	13.1590777669	8.1654531212
H62	3.0258015267	11.2198618291	8.6617138726
N63	5.2296975840	13.5531128733	8.2389162578
C64	6.1962671820	12.5161099458	8.5353112957
C65	5.4859360022	14.8542519221	8.8263083953
H66	3.3750443192	13.1079469569	9.3826115188
H67	3.2835818239	14.0604338673	7.8324852566
H68	4.7272856867	15.5737377522	8.4710662987
H69	6.4812839815	15.2243573340	8.5216835127
H70	5.4457751010	14.8496949003	9.9364894996
H71	7.1728236199	12.7473963814	8.0725600024
H72	5.8156908879	11.5751832305	8.1084225354
H73	6.3645672024	12.3689562430	9.6261746073

Name – INT-B7\\G=-1853.815261\\H=-1853.709664\\SCF E(PBE-D3/BS2)=-1854.41132296606 \\ZeroPoint=393.849

Angstroms

Atom	x	y	z
Fe1	1.6487527422	12.3192699247	11.1490282748
O2	0.6727081367	14.3717880957	12.9355185887

P3	0.1545929912	12.6601155573	9.6004650362
N4	2.5300237165	10.9923987879	9.7376465778
C5	1.5731640646	10.4890919270	8.7189766257
H6	0.9079845626	9.7690735319	9.2242121930
H7	2.1161772332	9.9485792372	7.9161282532
C8	0.7664387998	11.6529490484	8.1464428560
H9	-0.0471578050	11.2999335306	7.4897431943
H10	1.4244895679	12.3059190507	7.5454996836
P11	3.1371128241	11.5320306705	12.5305630772
C12	-0.1434038330	14.3782850977	8.8584382054
H13	-0.7115391469	14.9097217543	9.6474219309
C14	1.1872428208	15.1181903557	8.6520934502
H15	1.7953562015	14.6343499842	7.8647543174
H16	1.7860209542	15.1147662946	9.5768779229
H17	1.0006194403	16.1598139208	8.3341200947
C18	-0.9767569673	14.3712736621	7.5641254389
H19	-1.1515912724	15.4069443702	7.2204725644
H20	-1.9643712061	13.8974850688	7.6902024955
H21	-0.4485663948	13.8400816944	6.7515592911
C22	-1.6161359457	12.0664860871	9.9022043982
H23	-2.2266559177	12.4173095085	9.0491299499
C24	-2.1421980565	12.6957400198	11.2018159991
H25	-2.1204561295	13.7985842195	11.1774999515
H26	-1.5196020283	12.3636225950	12.0500648983
H27	-3.1862116461	12.3836157560	11.3852056359
C28	-1.7062929616	10.5355240295	9.9697045968
H29	-1.4506882162	10.0559972786	9.0098381508
H30	-2.7353490354	10.2276048464	10.2291361012
H31	-1.0217992706	10.1521021306	10.7469245639
C32	3.2641904942	9.8623863353	10.3630575272
H33	3.8495815728	9.3141087735	9.5961196963
H34	2.5092881746	9.1709934665	10.7731549454
C35	4.1721683272	10.3837498562	11.4756429356
H36	4.9911532782	10.9842057220	11.0404925354
H37	4.6278944054	9.5581478624	12.0489662167
C38	2.5518643226	10.4770838372	13.9884360265
H39	3.4383361436	10.2682179944	14.6160435368
C40	1.9527228670	9.1405979195	13.5293654626
H41	1.1290423308	9.3225906322	12.8167461041
H42	1.5468146316	8.5895386580	14.3968512212
H43	2.6987898399	8.4890039259	13.0443361918
H44	0.7542442663	11.1111348002	11.5918738926
C45	1.5233580291	11.2765708527	14.8037344736
H46	1.9299774626	12.2305806903	15.1801262185
H47	1.1821244277	10.6892114450	15.6753746357
H48	0.6509547291	11.5074313672	14.1689726850
C49	4.4177277869	12.6480645217	13.3710532011
H50	3.8393721195	13.1527695546	14.1695424635
C51	4.9255614865	13.7249269445	12.4012342109
C52	5.5915986176	11.8874214436	14.0122947702
H53	6.1898140404	11.3611749131	13.2475109946
H54	5.2663447177	11.1430620143	14.7569783110

H55	6.2663000001	12.5942992835	14.5280254825
C56	1.0533640902	13.5017561149	12.2113895893
O57	4.6482414326	12.3556150989	8.1822237011
C58	4.7680362499	13.5184810033	8.6293689486
H59	3.2348929655	11.5640917957	9.2310725909
N60	5.7337051202	14.3972877640	8.2605601394
C61	6.7455789153	14.0345796295	7.2747510563
C62	5.8071608054	15.7300151457	8.8470581634
H63	2.6067852691	13.3907705198	10.5883869850
H64	4.0597824186	13.9125290168	9.3917291571
H65	6.7086737774	14.7242221046	6.4127987330
H66	6.5437830165	13.0097498626	6.9329434371
H67	7.7550672525	14.0807998644	7.7208219173
H68	4.9895009488	15.8620500940	9.5733106707
H69	5.7159909020	16.5070760834	8.0665854786
H70	6.7701489584	15.8718073754	9.3704660637
H71	5.5272288755	13.2783612591	11.5882822667
H72	5.5719645033	14.4462728431	12.9327695665
H73	4.0841610894	14.2582088907	11.9320665448

Name – TS-B2\\G=-1853.785418\\H=-1853.683639\\SCF E(PBE-D3/BS2)=-1854.39133249392\\ZeroPoint=397.468

Angstroms

Atom	x	y	z
Fe1	2.1024308887	12.3540287387	10.7024982779
O2	1.8126643527	14.8603540713	12.1259443503
P3	0.2927511368	12.6146937975	9.4734790676
N4	2.4352627382	10.6223748884	9.5253817219
C5	1.2509658003	10.1342090984	8.7679104847
H6	0.6040377319	9.5791548894	9.4672373715
H7	1.5746025972	9.4260529880	7.9776979276
C8	0.4999962495	11.3155761393	8.1466796937
H9	-0.4520267397	10.9981150989	7.6877916817
H10	1.1322164630	11.7689899435	7.3628104865
P11	3.5147130748	11.4330704487	12.1239515289
C12	-0.1980138253	14.2099829392	8.5746553791
H13	-0.7617548900	14.7569023252	9.3552489283
C14	1.0071858430	15.0723312514	8.1788162996
H15	1.5132659924	14.6560093040	7.2912140348
H16	1.7437351315	15.1363883034	8.9957684638
H17	0.6777217738	16.0925675976	7.9150275466
C18	-1.1306855077	13.9715942026	7.3741273784
H19	-1.4793431423	14.9381310773	6.9682954556
H20	-2.0252776331	13.3817163052	7.6341647687
H21	-0.6019733086	13.4446159746	6.5610750381
C22	-1.3665025074	12.2534310879	10.3135911040
H23	-2.1435287661	12.5709961829	9.5922987160

C24	-1.4913172687	13.1029174397	11.5895190042
H25	-1.3611265913	14.1819006512	11.4002857444
H26	-0.7219448523	12.7971050336	12.3180999091
H27	-2.4865814259	12.9604804606	12.0469180344
C28	-1.5785993504	10.7677300943	10.6323018901
H29	-1.6077388230	10.1413039207	9.7255593717
H30	-2.5392580440	10.6298177630	11.1605221474
H31	-0.7749920776	10.3955655669	11.2916346208
C32	3.1351269961	9.4956344244	10.1966015856
H33	3.5688280411	8.8147329728	9.4357379584
H34	2.3839955821	8.9193603069	10.7614460121
C35	4.2302402791	10.0135043473	11.1336446852
H36	5.0628681711	10.4287494668	10.5403768464
H37	4.6345880583	9.2018487046	11.7630706444
C38	2.7637693602	10.6289879557	13.6713000738
H39	3.6303859037	10.3347404705	14.2958836889
C40	1.9247474911	9.3777844980	13.3843567784
H41	1.1065360559	9.6130412207	12.6813597636
H42	1.4680576209	9.0080029492	14.3201619601
H43	2.5254786001	8.5545040008	12.9639730010
H44	1.1176782303	11.5886714397	11.5638897467
C45	1.9272414958	11.6745880680	14.4281248571
H46	2.4974958865	12.5877771618	14.6705633764
H47	1.5524472195	11.2518429516	15.3771980607
H48	1.0642514552	11.9762456711	13.8105718238
C49	4.9812531501	12.2719419425	13.0072985534
H50	4.5635918124	12.4774720548	14.0112298917
C51	5.3886819651	13.6186901776	12.4018971886
H52	4.5216840088	14.2840133331	12.2733884206
H53	5.8618608579	13.4924264056	11.4170577134
H54	6.1196150080	14.1214143264	13.0608255271
C55	6.1890997551	11.3361423829	13.1820628837
H56	6.6697457191	11.1136354268	12.2133473811
H57	5.9167198444	10.3764516011	13.6533265625
H58	6.9489244846	11.8169464173	13.8237202945
C59	1.9334760111	13.8284463448	11.5425524636
O60	3.8594502786	11.7655815024	7.5777211656
C61	3.9274417072	12.9755839046	8.0170983725
H62	3.0907201421	11.0212643511	8.7866931064
N63	5.1847115579	13.5843869888	8.2388758460
C64	6.2537984713	12.7013287788	8.6773604827
C65	5.1266767872	14.9007893515	8.8603354873
H66	3.2961802989	13.0284542157	9.4394073171
H67	3.2101049550	13.7364252216	7.6464430059
H68	4.4346310663	15.5474435652	8.2937586938
H69	6.1232902166	15.3706469534	8.8472099065
H70	4.7600174663	14.8461450487	9.9068021031
H71	7.2275864782	13.2069769204	8.5720027474
H72	6.2379628935	11.7956759285	8.0532123100
H73	6.1325901253	12.3878501294	9.7368836911

Name – INT-A7\\G=-1605.663588\\H=-1605.574865\\SCF E(PBE-D3/BS2)=-1606.15780794580\\ZeroPoint=330.866

Angstroms

Atom	x	y	z
Fe1	1.9351556916	11.8126370711	10.9414992632
O2	-0.2509695210	11.4564915042	12.8433464634
P3	0.8040390815	12.5252164983	9.2197275885
N4	2.1262683322	10.0127023156	9.8750071321
C5	0.9588019770	9.7780110618	8.9853919837
H6	0.0870311728	9.6176609002	9.6421562873
H7	1.1060484210	8.8639525546	8.3738088619
C8	0.7505054143	11.0102878486	8.0972935650
H9	-0.1889167423	10.9372210652	7.5237614979
H10	1.5744117130	11.0873893625	7.3654080618
P11	3.6163949857	11.0320884843	12.0957064578
C12	1.4946493216	13.9077303604	8.1140756500
H13	1.5810248425	14.7614395846	8.8135126125
C14	2.9063427370	13.5800502212	7.6044984130
H15	2.8896679399	12.7707897692	6.8518088939
H16	3.5657492671	13.2693277113	8.4297486160
H17	3.3466815607	14.4690629992	7.1193345197
C18	0.5835151763	14.3075868869	6.9391612442
H19	1.0952780224	15.0533030574	6.3047053764
H20	-0.3656242851	14.7595183745	7.2675354345
H21	0.3464001212	13.4397806728	6.2974925902
C22	-1.0125983502	13.0236326171	9.3626857247
H23	-1.3382941777	13.3148637134	8.3475948155
C24	-1.1305226005	14.2352152824	10.3008280172
H25	-0.5545978100	15.1018762509	9.9341912882
H26	-0.7522672431	13.9799268478	11.3048891312
H27	-2.1853565574	14.5494197154	10.3968356961
C28	-1.9095548390	11.8649878224	9.8236888308
H29	-1.8864987891	11.0139397510	9.1224961857
H30	-2.9572944382	12.2115752102	9.8822693403
H31	-1.6208353987	11.5006441142	10.8203915731
C32	2.4026412407	8.8866331194	10.8075513063
H33	2.5154762764	7.9320850596	10.2531512009
H34	1.5209165406	8.8058475036	11.4651355623
C35	3.6603907378	9.1979289519	11.6295641268
H36	4.5687601411	8.9965571004	11.0356500919
H37	3.7149564212	8.5540511112	12.5227508700
C38	3.6673345654	11.0228130053	13.9801764631
H39	4.5902411502	10.4826185516	14.2626887298
C40	2.4711161428	10.2810580371	14.5938016549
H41	1.5269319204	10.8060299261	14.3883031331
H42	2.5967279175	10.2217794645	15.6900845225
H43	2.3732775356	9.2487700630	14.2163083811
H44	2.9512471431	10.1209110108	9.2657905137
C45	3.7440861162	12.4694942076	14.4939248812

H46	4.6468805110	12.9931466580	14.1378195012
H47	3.7597186646	12.4869263496	15.5981312281
H48	2.8651087897	13.0418695115	14.1510266805
C49	5.3676189107	11.6258003622	11.6533091887
H50	5.3021125572	12.7189566988	11.8112686916
C51	5.6728696870	11.3876549986	10.1654607751
H52	4.8362184963	11.7233285231	9.5308636921
H53	5.8683838943	10.3209394852	9.9533258879
H54	6.5766964854	11.9481820676	9.8687478918
C55	6.4916976043	11.0489473697	12.5296979279
H56	6.5016850024	9.9443949574	12.4974172940
H57	6.4135260222	11.3582627249	13.5837963188
H58	7.4733574640	11.3950441259	12.1592901818
C59	0.6370009928	11.5127794370	12.0425909605
H60	3.0665123124	12.4532596053	10.1337056075
H61	2.0150466853	13.1845600269	11.5644296453

Name – INT-B4\\G=-1605.674657\\H=-1605.576888\\SCF E(PBE-D3/BS1)=-1606.13431920953 \\ZeroPoint=330.258

Angstroms

Atom	x	y	z
Fe1	2.3479418966	11.9555835563	10.6074675387
P2	0.7544336138	12.5032346231	9.2282207901
N3	2.1390725630	10.0018169199	9.7928716043
C4	0.8110152255	9.7604908556	9.1632023457
H5	0.0904328341	9.6602837531	9.9916644838
H6	0.8185166954	8.8051228716	8.5999227223
C7	0.4196101816	10.9318847375	8.2640421977
H8	-0.6311807276	10.8467195495	7.9373268855
H9	1.0491528128	10.9479151932	7.3571901059
P10	3.6561396733	11.0095287181	12.0684972073
C11	1.0367559775	13.8166705003	7.8932966765
H12	1.2169629025	14.7381057049	8.4804098927
C13	2.3190642452	13.5064939661	7.1061800565
H14	2.1727873395	12.6508450126	6.4222378485
H15	3.1441777375	13.2575675633	7.7933370201
H16	2.6074444078	14.3745394679	6.4874316126
C17	-0.1544786428	14.0483318826	6.9487633808
H18	0.1172031542	14.7833788904	6.1698547324
H19	-1.0427713825	14.4394522497	7.4698221093
H20	-0.4449991932	13.1157442787	6.4326725778
C21	-0.9329080353	12.9944338802	9.9236147248
H22	-1.5800626205	13.2239366604	9.0573555721
C23	-0.7703842906	14.2507892896	10.7930405015
H24	-0.3547314138	15.1030049943	10.2292467011
H25	-0.0897363676	14.0368601593	11.6340633491
H26	-1.7461435667	14.5643506007	11.2048004651
C27	-1.5828101627	11.8575344726	10.7241119067
H28	-1.8358983477	10.9901969759	10.0909073464
H29	-2.5203157160	12.2119084432	11.1894405408
H30	-0.9003233635	11.5196109186	11.5233554084

C31	2.4546801808	8.9157251228	10.7622088720
H32	2.5135693809	7.9387535370	10.2406524088
H33	1.6068298154	8.8741471081	11.4659161338
C34	3.7486998890	9.2220964306	11.5142978795
H35	4.6183640265	9.1192351432	10.8420052214
H36	3.8935473603	8.5209613477	12.3543485847
C37	3.0993968022	10.9133195045	13.8721734944
H38	3.9039807748	10.3974430339	14.4273248666
C39	1.8053908791	10.1047084425	14.0362800098
H40	1.0136477221	10.5233238236	13.3906871644
H41	1.4631888653	10.1490768155	15.0861222850
H42	1.9404707348	9.0407068700	13.7779248116
H43	2.8527916429	9.9851330066	9.0509230223
C44	2.9261615412	12.3380713145	14.4203577987
H45	3.8576380002	12.9264019850	14.3665832648
H46	2.6076145544	12.3092525452	15.4778284399
H47	2.1552159437	12.8701040749	13.8381512475
C48	5.4670492854	11.5389283145	12.2344557641
H49	5.3931662265	12.5886596458	12.5794511786
C50	6.1467685348	11.5468893160	10.8571462034
H51	5.5102012924	12.0543002960	10.1141880231
H52	6.3375419249	10.5187243147	10.4993914983
H53	7.1225914533	12.0607531425	10.9149275194
C54	6.2869128753	10.7321365311	13.2546833526
H55	6.2817884722	9.6546561105	13.0110578761
H56	5.9186226076	10.8492071474	14.2860549904
H57	7.3399240411	11.0661209782	13.2437874618
H58	1.1972078453	11.5821316234	11.5874096472
H59	3.4769764610	12.1402236489	9.5541587597
C60	2.6467540673	13.5393372290	11.1365043329
O61	2.8918900966	14.6567753726	11.4751168549

Name – Trans-DhB\\G=-1721.223011\\H=-1721.129702\\SCF E(PBE-D3/BS1)=-1721.74362825560\\ZeroPoint=363.188

Angstroms

Atom	x	y	z
Fe1	2.4150372399	11.8882649760	10.5695998039
P2	0.8071238097	12.4290343923	9.1927843823
N3	2.1015587779	9.9002658568	9.8921383179
C4	0.7558336839	9.6870068193	9.2933065802
H5	0.0307029673	9.6724432786	10.1235775002
H6	0.7137529038	8.7014277697	8.7855949048
C7	0.4352186199	10.8187651671	8.3163094365
H8	-0.6010692661	10.7516518350	7.9438161014
H9	1.1144094606	10.7649594695	7.4474358850
P10	3.6911233613	10.9777382384	12.0899447339
C11	1.0297457214	13.6946853959	7.8021872285
H12	0.8050990704	14.6589916865	8.2985399594
C13	2.4798165969	13.7428257634	7.3017197340

H14	2.7778011566	12.7871123122	6.8369153143
H15	3.1767224014	13.9273310447	8.1332843136
H16	2.5946243881	14.5426458190	6.5483151722
C17	0.0402222845	13.5019909338	6.6397947504
H18	0.1222240448	14.3435347780	5.9288901159
H19	-1.0096513597	13.4525845513	6.9740978917
H20	0.2597589745	12.5769157240	6.0790566901
C21	-0.8380257694	13.0203526920	9.9131438614
H22	-1.4409943651	13.3825771343	9.0582164232
C23	-0.5746871555	14.1876519925	10.8784872001
H24	-0.0364201996	15.0233030189	10.3992684232
H25	0.0379938280	13.8342507173	11.7253065022
H26	-1.5285619457	14.5836692894	11.2708380328
C27	-1.6093631406	11.8997824288	10.6235411080
H28	-1.9064092746	11.0893256649	9.9369977156
H29	-2.5326151940	12.3039496578	11.0763159708
H30	-0.9922086209	11.4678791045	11.4310879100
C31	2.4017413647	8.8601818858	10.9115440864
H32	2.4217624906	7.8552793985	10.4421195210
H33	1.5735555521	8.8745269016	11.6388476240
C34	3.7261154734	9.1680069015	11.6111070330
H35	4.5708512789	9.0293346236	10.9117447326
H36	3.8922264828	8.4940528670	12.4691979911
C37	3.1066387437	11.0179819193	13.8875513420
H38	3.9308425378	10.6105579210	14.5022327075
C39	1.8569507938	10.1566446844	14.1160424207
H40	1.0442140761	10.4814209935	13.4428001054
H41	1.5073338935	10.2671658847	15.1581487438
H42	2.0479117863	9.0838749872	13.9454775156
H43	2.7876430739	9.8053996886	9.1201832020
C44	2.8397644110	12.4757576837	14.2944631758
H45	3.7268427682	13.1197927574	14.1717290159
H46	2.5311545219	12.5278494991	15.3538632411
H47	2.0307797432	12.8910789960	13.6698966241
C48	5.5153933111	11.4419847578	12.2927588161
H49	5.4735310673	12.4171260884	12.8165537088
C50	6.1865182967	11.6620673353	10.9296541740
H51	5.5920745202	12.3394413368	10.2975711988
H52	6.2941894492	10.7083050065	10.3817190093
H53	7.2002709284	12.0793729833	11.0655338583
C54	6.3228569050	10.4526765989	13.1520047312
H55	6.3804970783	9.4606216774	12.6701073817
H56	5.9019358649	10.3140399566	14.1612432237
H57	7.3581253637	10.8180504571	13.2762223035
H58	1.2678683653	11.6352904508	11.5828117177
H59	3.5748967335	12.0317580304	9.5196259357
C60	2.7601876769	13.4928503764	11.0136464315
O61	3.7658796414	10.5498585202	7.5852036451
C62	5.1550395346	10.2858709992	7.3914800063
H63	3.6906387873	11.2405304432	8.3249913213
H64	5.2548030267	9.5899903460	6.5411391020
H65	5.6258161048	9.8124207445	8.2765962713

H66	5.7270178129	11.2035736411	7.1520982936
O67	3.0371550192	14.6197190559	11.2831345236

Name – Trans-DhC\\G=-1721.204852\\H=-1721.112034\\SCF E(PBE-D3/BS1)=-1721.72192201301\\ZeroPoint=360.530

Angstroms

Atom	x	y	z
Fe1	2.4128822802	12.0762083706	10.5379867723
P2	0.7471189514	12.5445206155	9.1661349062
N3	2.2676608383	10.1626888525	9.7560463142
C4	1.0436345313	9.8533833935	9.0094222924
H5	0.2022318178	9.6110523277	9.6981670805
H6	1.1997751493	8.9424988896	8.3879338169
C7	0.6381291015	11.0202301640	8.1106828393
H8	-0.3559059259	10.8818390526	7.6521463381
H9	1.3785814574	11.1486105266	7.3005508734
P10	3.6728215289	11.1070668063	12.0879099561
C11	0.8687567412	13.9762927002	7.9409719467
H12	0.5765126998	14.8665144997	8.5300543519
C13	2.3115059665	14.1761768229	7.4515152510
H14	2.6940740033	13.2742673851	6.9390902875
H15	2.9927663351	14.4102893439	8.2844903907
H16	2.3561098016	15.0106579849	6.7285443613
C17	-0.1038964164	13.8231632855	6.7580597823
H18	-0.0744654433	14.7302798007	6.1304148909
H19	-1.1483405470	13.6759976717	7.0779937668
H20	0.1768567680	12.9696541651	6.1182592353
C21	-0.9544871312	12.8330388653	9.9214224857
H22	-1.6033257035	13.1591790236	9.0863676825
C23	-0.8752955240	13.9572651188	10.9671489286
H24	-0.4476085466	14.8899393183	10.5628919473
H25	-0.2496119875	13.6390573938	11.8170033960
H26	-1.8851808312	14.1895380216	11.3474748388
C27	-1.5520357229	11.5600477900	10.5384675613
H28	-1.7502420987	10.7799786906	9.7855088270
H29	-2.5116139294	11.7988784257	11.0319820050
H30	-0.8717178297	11.1420133702	11.3013189605
C31	2.4746922696	9.0864771370	10.7294931758
H32	2.5565486505	8.1093731053	10.2015274246
H33	1.6073353910	8.9914030451	11.4228345453
C34	3.7526451714	9.3388399574	11.5255151855
H35	4.6231893571	9.2665616187	10.8509113220
H36	3.8939520077	8.6310099450	12.3591433052
C37	3.0277655823	11.0744044103	13.8571754292
H38	3.8318824191	10.6091908010	14.4585601708
C39	1.7587448138	10.2210313012	13.9962732445
H40	0.9630154545	10.6014708466	13.3328268573
H41	1.3884880902	10.2674773516	15.0358027367

H42	1.9344521081	9.1608528275	13.7525650530
H43	3.5753979197	10.1513020821	8.7953922066
C44	2.7823615393	12.5036084264	14.3665035878
H45	3.6692878184	13.1515535819	14.2675129964
H46	2.5028694354	12.4800299730	15.4344700094
H47	1.9572874103	12.9726568712	13.8067628040
C48	5.4817098933	11.5970204444	12.3278390395
H49	5.4476974405	12.4946764043	12.9744623343
C50	6.1249078107	11.9840735929	10.9859697040
H51	5.6871844421	12.9130123423	10.5867481904
H52	5.9908138987	11.1963133937	10.2219774529
H53	7.2084528707	12.1501614211	11.1187105113
C54	6.2985950384	10.5040342787	13.0424564441
H55	6.4152378636	9.6113969993	12.4046510926
H56	5.8459594340	10.1825683118	13.9948338054
H57	7.3113647415	10.8817738881	13.2692761803
H58	3.2965944016	12.4062017742	9.1754499127
C59	2.5243949737	13.6705579703	11.1902086716
O60	4.4417910375	10.0876081189	8.2137869384
C61	4.5673123593	8.7254098739	7.8533799712
H62	3.8625595359	12.1288818061	9.7347730372
H63	3.6873484248	8.3355277833	7.2930223241
H64	4.7149463208	8.0518539351	8.7285103473
H65	5.4490594998	8.5972259578	7.1996017753
O66	2.5732566832	14.7646922921	11.6429789051
H67	1.3125542979	11.7135227093	11.4778915414

Name – Trans-DhD\\G=-1720.054941\\H=-1719.959409\\SCF E(PBE-D3/BS1)=-1720.55253110456\\ZeroPoint=349.878

Angstroms

Atom	x	y	z
Fe1	2.3274378880	11.8826892168	10.6015223010
O2	3.3160893248	14.5911839987	10.9986739067
P3	0.7904297250	12.4508334311	9.1388175200
N4	2.1134835176	10.1340854315	9.9397500004
C5	1.0127997538	9.7331200907	9.0372506423
H6	0.1518356092	9.3734845180	9.6404024108
H7	1.3309987781	8.8688407156	8.4145534568
C8	0.5847768575	10.8938506343	8.1365770613
H9	-0.4381617267	10.7691856978	7.7429842585
H10	1.2778569755	10.9683449724	7.2812535452
P11	3.6758013857	10.9936082080	12.0794332936
C12	1.1729810278	13.7960374782	7.8799276035
H13	1.1398535834	14.7339308828	8.4667550926
C14	2.6081861010	13.6174776328	7.3560845568
H15	2.7346533810	12.6672816651	6.8109583930
H16	3.3345039179	13.6141124061	8.1839721586
H17	2.8643185637	14.4418706969	6.6674081502
C18	0.1510121906	13.8822797853	6.7353188451

H19	0.4227416187	14.7019235971	6.0464178485
H20	-0.8717097815	14.0796252155	7.0960257617
H21	0.1316053797	12.9494981057	6.1451221973
C22	-0.9240011920	12.8744380945	9.7822673605
H23	-1.5713192123	13.0296595457	8.8978598481
C24	-0.8706109449	14.1670421240	10.6122087313
H25	-0.5402254010	15.0351306619	10.0174744153
H26	-0.1724011522	14.0482681987	11.4592264636
H27	-1.8707694891	14.4012591502	11.0183293501
C28	-1.4812555149	11.7033709634	10.6083261731
H29	-1.6429450864	10.8009121622	9.9959524484
H30	-2.4522231562	11.9817630284	11.0558470176
H31	-0.7844540601	11.4442286977	11.4246240510
C32	2.5704564909	8.9323913268	10.6707634848
H33	2.7814588553	8.1103956351	9.9535034668
H34	1.7477078807	8.5633774424	11.3208565557
C35	3.8141534109	9.2229278702	11.5146204148
H36	4.7248167990	9.1476913329	10.8957322908
H37	3.9237734457	8.5175342697	12.3560078253
C38	3.1168673564	10.9049960982	13.8699202917
H39	3.8809941996	10.3196913202	14.4167313892
C40	1.7674876095	10.1738042612	13.9640424895
H41	1.0137768243	10.6773487940	13.3338058034
H42	1.4059283406	10.1765610512	15.0079260472
H43	1.8386274580	9.1226585345	13.6385405469
H44	3.4113907468	10.4856375340	8.4957429865
C45	3.0295573206	12.3199706965	14.4633883802
H46	4.0056375722	12.8337411443	14.4693810635
H47	2.6684857604	12.2748446795	15.5060770877
H48	2.3235202944	12.9362971187	13.8796927291
C49	5.4456061983	11.6300290064	12.1507739212
H50	5.3389556996	12.6618885867	12.5377315692
C51	6.0106219735	11.7221736572	10.7213433614
H52	5.3224281104	12.2687176839	10.0537455590
H53	6.1767778920	10.7212310209	10.2819648783
H54	6.9843362030	12.2431426841	10.7309197211
C55	6.3684673400	10.8312442008	13.0846970769
H56	6.4454345218	9.7757185506	12.7666659213
H57	6.0237846072	10.8480333616	14.1321294479
H58	7.3878443508	11.2564542959	13.0648250289
C59	2.9110121773	13.4829833279	10.8335858610
H60	1.3748308486	12.1882496995	11.6842789664
O61	3.9520602565	10.4373040213	7.6609156476
C62	4.5267476383	9.1353997759	7.6141175698
H63	3.7660580818	8.3281603293	7.5568983332
H64	5.1814744312	8.9171441763	8.4833763709
H65	5.1517765121	9.0649140016	6.7080640464

Name – Trans-TS-Dh1\\G=-1721.199986\\H=-1721.112972\\SCF E(PBE-D3/BS1)=-1721.70658041943\\ZeroPoint=360.552

Angstroms

Atom	x	y	z
Fe1	2.5098545229	11.9440940804	10.5199716516
P2	0.8199998834	12.4608270884	9.1803837005
N3	2.1953751386	10.0092465396	9.8383281305
C4	0.8248905277	9.7519507186	9.3745619240
H5	0.1136603713	9.7011571376	10.2292501370
H6	0.7806322487	8.7605928213	8.8697630925
C7	0.3879891954	10.8377715411	8.3907256964
H8	-0.6786349926	10.7705483883	8.1196295339
H9	0.9895009722	10.7633790491	7.4693498633
P10	3.7351046211	10.9801475933	12.0815586647
C11	1.0714934990	13.6437939826	7.7292593028
H12	1.0023639190	14.6539071405	8.1744809524
C13	2.4750030626	13.4690745307	7.1254010182
H14	2.6777184949	12.4136107305	6.8656587971
H15	3.2561159885	13.7984118480	7.8284251967
H16	2.5703187109	14.0723471009	6.2047610824
C17	-0.0195251094	13.5036749765	6.6521965209
H18	0.1021072282	14.2929474292	5.8899204412
H19	-1.0383414373	13.5945065758	7.0584182358
H20	0.0539738587	12.5332270453	6.1363029413
C21	-0.7676595500	13.0994649993	9.9643160640
H22	-1.4382264268	13.3438578567	9.1181375169
C23	-0.4994350054	14.3759562311	10.7772289504
H24	0.0015456281	15.1615591187	10.1866692705
H25	0.1368333947	14.1499784371	11.6486593923
H26	-1.4523877664	14.7925280495	11.1486194611
C27	-1.4482804497	12.0324740692	10.8344628020
H28	-1.7580187426	11.1485748504	10.2536717785
H29	-2.3528878938	12.4552815363	11.3067723790
H30	-0.7678925485	11.6972032522	11.6368341976
C31	2.5627584774	8.9215360825	10.7542510972
H32	2.6677883810	7.9713207747	10.1845541579
H33	1.7588320779	8.7431103545	11.5018826831
C34	3.8676443358	9.2243527708	11.4906351882
H35	4.7228038634	9.1931677842	10.7918193295
H36	4.0700637647	8.5099208870	12.3067431204
C37	3.0321768826	10.9301108042	13.8284815529
H38	3.8401000714	10.5246608626	14.4665612548
C39	1.8071342042	10.0130706403	13.9473279804
H40	1.0182879216	10.3270641836	13.2423075807
H41	1.3929943167	10.0728924404	14.9695705220
H42	2.0505110434	8.9573141091	13.7486356344
H43	2.9625374236	9.9535976491	8.4685716286
C44	2.6912323513	12.3542489196	14.2943168941
H45	3.5461032231	13.0465726598	14.2191569920
H46	2.3655503867	12.3370895340	15.3492048570
H47	1.8702989559	12.7649571322	13.6840675638
C48	5.5101991802	11.5340335377	12.4161979116

H49	5.3965626550	12.3954650285	13.1013696149
C50	6.2019724496	12.0276978307	11.1376748071
H51	5.6672795445	12.8810742245	10.6917938007
H52	6.2654807690	11.2293106274	10.3772099617
H53	7.2334898056	12.3510797179	11.3641267283
C54	6.3469852837	10.4501595309	13.1203137579
H55	6.5291753867	9.5921608486	12.4523507198
H56	5.8689480737	10.0687100939	14.0366671580
H57	7.3304642947	10.8607809774	13.4074793739
H58	1.4080177160	11.7190882697	11.4989695489
H59	3.9463847083	11.9551972267	9.6930646659
C60	2.7585091682	13.5509353864	11.0984048115
O61	3.3547199147	9.9058528192	7.4901861290
C62	4.7526069018	10.0882214098	7.5746447585
H63	3.3558090982	12.0400881215	9.1004074070
H64	5.2665327870	9.5357245276	6.7616840405
H65	5.1804124969	9.7159500306	8.5320239227
H66	5.0571832839	11.1575381087	7.4884932820
O67	2.9239678437	14.6440520131	11.5246987954

Name – Trans-TS-Dh2\\G=-1721.203288\\H=-1721.108649\\SCF E(PBE-D3/BS1)=-1721.71583205730\\ZeroPoint=358.655

Angstroms

Atom	x	y	z
Fe1	2.4111725764	12.0807929203	10.5426172701
P2	0.7504469071	12.5567641821	9.1607941238
N3	2.2509393018	10.1746048414	9.7707593291
C4	1.0467828277	9.8537382309	8.9918936637
H5	0.1978370934	9.5805056580	9.6586092801
H6	1.2338588462	8.9579207360	8.3572915912
C7	0.6354186500	11.0295424353	8.1041191729
H8	-0.3608383578	10.8916282607	7.6500782016
H9	1.3696061459	11.1627580292	7.2889276343
P10	3.6801862927	11.1054688529	12.0859403088
C11	0.8334757140	13.9940418207	7.9337171384
H12	0.5305447376	14.8745918194	8.5318897309
C13	2.2660720335	14.2295781819	7.4322196678
H14	2.6583305833	13.3477195304	6.8936491638
H15	2.9523725606	14.4576380077	8.2631951253
H16	2.2876450019	15.0805202602	6.7286429014
C17	-0.1476165945	13.8315576938	6.7587071012
H18	-0.1439431730	14.7445762625	6.1372777018
H19	-1.1856848884	13.6605469379	7.0882580096
H20	0.1447225784	12.9888283442	6.1088720615
C21	-0.9456723601	12.8352138013	9.9348206943
H22	-1.6095647421	13.1533989137	9.1084359818
C23	-0.8607694030	13.9645125652	10.9753385637
H24	-0.4529321565	14.9007292674	10.5584946722
H25	-0.2123191935	13.6587590521	11.8133936437
H26	-1.8659973689	14.1864310795	11.3753614986

C27	-1.5237074088	11.5586499230	10.5631204327
H28	-1.7275322864	10.7770210618	9.8134078466
H29	-2.4769687378	11.7897184599	11.0717857178
H30	-0.8285946614	11.1457353203	11.3149952431
C31	2.4795621120	9.0783120598	10.7214895337
H32	2.5755314969	8.1139280980	10.1733939716
H33	1.6158534687	8.9532087394	11.4133292858
C34	3.7576326546	9.3351977439	11.5198519626
H35	4.6286452623	9.2667332055	10.8447276049
H36	3.9007465810	8.6241565698	12.3507885458
C37	3.0189424284	11.0717130153	13.8504580376
H38	3.8218357816	10.6188463754	14.4629469401
C39	1.7568899088	10.2070050257	13.9839077330
H40	0.9611988513	10.5762777482	13.3137093222
H41	1.3776875784	10.2542837042	15.0205945995
H42	1.9451776050	9.1477226378	13.7457718413
H43	3.5930191430	10.1282669730	8.7869413951
C44	2.7553718611	12.5019080912	14.3480543628
H45	3.6388053712	13.1557074888	14.2567711902
H46	2.4610493881	12.4839917902	15.4124509668
H47	1.9357397522	12.9612133602	13.7715421871
C48	5.4894394643	11.5850683712	12.3641662505
H49	5.4415242047	12.4659380585	13.0326534890
C50	6.1549791453	12.0122758338	11.0459857699
H51	5.6993421836	12.9344175602	10.6510301945
H52	6.0641202578	11.2304066386	10.2693302275
H53	7.2306350791	12.2067644124	11.2061103552
C54	6.2982675126	10.4776546475	13.0641319933
H55	6.4232964334	9.5992531660	12.4080434603
H56	5.8333932631	10.1351152646	14.0034550023
H57	7.3080424156	10.8506069136	13.3118930652
H58	3.5352139263	12.4656025764	8.9702169735
C59	2.5752870008	13.6842873514	11.1578992253
O60	4.4486818800	10.0177193371	8.2120939347
C61	4.5465521853	8.6397254494	7.9020159643
H62	4.0695401247	12.1585499462	9.4631128604
H63	3.6544545234	8.2453805660	7.3672298376
H64	4.6953866294	7.9970743862	8.7994054009
H65	5.4182108657	8.4771082784	7.2415165019
O66	2.6508636452	14.7854719114	11.5964767613
H67	1.3260340837	11.7932061403	11.5075378177

Name – Cis-DhB\\G=-1721.219159 \\H=-1721.124427\\SCF E(PBE-D3/BS1)=-1721.73852521013\\ZeroPoint=363.839

Angstroms

Atom	x	y	z
Fe1	2.1289385357	11.8321043017	10.8222141256
O2	0.0919435128	12.0448461981	12.8957553793
P3	0.8274687264	12.4465460400	9.1607872716
N4	1.9593047685	9.8851884164	10.0441489607

C5	0.6622509427	9.6936654957	9.3494832905
H6	-0.1355363583	9.7524196796	10.1090536238
H7	0.6150235946	8.6928697196	8.8717622145
C8	0.5162009645	10.8037003728	8.2984572785
H9	-0.4576594082	10.7566506568	7.7835328103
H10	1.3105192452	10.6864093980	7.5402527897
P11	3.6951676772	10.9997248524	12.1159178577
C12	1.3478137761	13.6490479312	7.7834425792
H13	1.0005840801	14.6244602586	8.1755308034
C14	2.8635280391	13.7420520275	7.5755533812
H15	3.2589134675	12.8020879669	7.1558865482
H16	3.3853180122	13.9343078669	8.5254195240
H17	3.0976650978	14.5559008132	6.8657259612
C18	0.6285405191	13.3787527744	6.4488784146
H19	0.8371800567	14.1961364191	5.7356151775
H20	-0.4667374265	13.3054383597	6.5550172974
H21	0.9867415499	12.4418343651	5.9883412399
C22	-0.9041983156	13.1468311552	9.4760579641
H23	-1.2773869311	13.4629040014	8.4827222532
C24	-0.8141960605	14.3894057280	10.3795656879
H25	-0.1228252709	15.1507029118	9.9802735768
H26	-0.4647690486	14.1147801074	11.3870334642
H27	-1.8087801119	14.8608933366	10.4758950362
C28	-1.8894309083	12.1144585755	10.0450586408
H29	-2.0380212050	11.2578009363	9.3671900034
H30	-2.8766373322	12.5873593662	10.1960766742
H31	-1.5529298043	11.7325469654	11.0211522848
C32	2.2871133417	8.8637689127	11.0674225601
H33	2.2590199881	7.8433590729	10.6316421264
H34	1.5213692876	8.9226394412	11.8591993331
C35	3.6829716660	9.1821791086	11.6210728893
H36	4.4320530348	9.0512743543	10.8181559976
H37	3.9639098423	8.5042271768	12.4441028792
C38	3.5011552323	10.9792563897	13.9990290636
H39	4.4694330897	10.6179260670	14.3947284773
C40	2.4038457728	10.0226067950	14.4906388354
H41	1.4142752034	10.3127562838	14.1062086891
H42	2.3536722850	10.0529901126	15.5939769437
H43	2.5973594173	8.9763376198	14.2018161518
H44	2.6897520439	9.8118671627	9.3153817288
C45	3.2685420392	12.4102247160	14.5148365085
H46	4.0617745532	13.1061460950	14.1934215820
H47	3.2470118411	12.4157637077	15.6195000585
H48	2.3077127392	12.8053655522	14.1499277911
C49	5.5215545581	11.5104200822	12.0258305803
H50	5.5715267143	12.3704129555	12.7212679383
C51	5.9375585174	12.0028868629	10.6364025747
H52	5.2780632880	12.8085577729	10.2810765103
H53	5.8909063237	11.1826737661	9.8996040713
H54	6.9797853026	12.3691754108	10.6565816685
C55	6.4858804936	10.4185057593	12.5259172613
H56	6.5189510031	9.5659128406	11.8248821015

H57	6.2194539428	10.0260294730	13.5213577735
H58	7.5108014022	10.8252778549	12.5959196515
C59	0.9057438198	11.8876331058	12.0346475152
H60	3.2879553038	12.1307190008	9.8298550865
H61	2.4763328466	13.2553929926	11.1804499965
O62	3.8266943111	10.5205972245	7.8970202678
C63	5.1123481804	10.5190814946	7.2742815162
H64	3.7836572290	11.2326221265	8.5949216862
H65	5.0855599484	9.7747333395	6.4614341341
H66	5.9275622681	10.2375211244	7.9689457420
H67	5.3586685540	11.5035946316	6.8308767365

Name – Cis-DhC\\G=-1721.197081 \\H=-1721.099372\\SCF E(PBE-D3/BS1)=-1721.70900107176\\ZeroPoint=360.358

Angstroms

Atom	x	y	z
Fe1	2.1321847882	11.9294653346	10.8339286979
O2	0.0045902547	11.6165797723	12.7744792341
P3	0.7837044820	12.5059879480	9.1362070279
N4	2.1828125282	10.0879410517	9.9082064608
C5	0.9305197143	9.7860948069	9.2149787734
H6	0.0746819015	9.6866558535	9.9240758695
H7	1.0128700101	8.8131167044	8.6801443269
C8	0.6450115109	10.8987973074	8.2029447342
H9	-0.3193637813	10.7820409315	7.6816489658
H10	1.4513965717	10.9077241204	7.4487438187
P11	3.7358803919	11.0749759306	12.1501714001
C12	1.3601905495	13.7570183876	7.8341361638
H13	1.0794587930	14.7388545502	8.2602179065
C14	2.8830030910	13.7325814652	7.6136778262
H15	3.2668826105	12.7074030789	7.4599513821
H16	3.4241601657	14.1692682000	8.4674536549
H17	3.1386088772	14.3323965270	6.7223584453
C18	0.6170026039	13.5726581015	6.4954997257
H19	0.8568498190	14.4138720857	5.8216454016
H20	-0.4792866934	13.5413852756	6.6064091520
H21	0.9321687695	12.6451880213	5.9884201510
C22	-0.9682001678	13.1192965421	9.4598767307
H23	-1.3288069122	13.4937961144	8.4831305367
C24	-0.9371663423	14.2978437965	10.4487671144
H25	-0.2617591759	15.1047631283	10.1177497833
H26	-0.6016718552	13.9671784683	11.4444117599
H27	-1.9486121673	14.7293900130	10.5519906528
C28	-1.9273528460	12.0113673819	9.9236072840
H29	-2.0092782044	11.1941360957	9.1889422009
H30	-2.9383992169	12.4351403464	10.0599731778
H31	-1.6164137260	11.5795127343	10.8867016366
C32	2.5278206797	9.0137524350	10.8394930224
H33	2.6039377206	8.0447580625	10.2965403602
H34	1.7472727307	8.8764135320	11.6249268754

C35	3.8749836316	9.3373394691	11.4915606433
H36	4.6500703897	9.3660683526	10.7057133555
H37	4.1798679476	8.6060741804	12.2582206098
C38	3.4943839702	10.9493821725	14.0145153059
H39	4.4870590903	10.6701418931	14.4158865571
C40	2.4938116722	9.8585774686	14.4291223982
H41	1.4846912933	10.0615111773	14.0399229697
H42	2.4241681360	9.8242482426	15.5311182556
H43	2.8013810458	8.8571295346	14.0869854205
H44	3.3464080058	10.3231427833	8.8807052424
C45	3.1102492099	12.3247120222	14.5881358104
H46	3.8295820294	13.1119960056	14.3059438238
H47	3.0813022817	12.2778960341	15.6912612233
H48	2.1156603898	12.6359739971	14.2315544210
C49	5.5049249083	11.7516556937	12.0720556985
H50	5.5056081677	12.5892989022	12.7949852677
C51	5.8768331779	12.2988706429	10.6829478188
H52	5.3588414308	13.2464904425	10.4675866403
H53	5.6301878980	11.5866575939	9.8740005326
H54	6.9616496644	12.5016267171	10.6433540328
C55	6.5374866112	10.7038763130	12.5344921284
H56	6.6353903477	9.8885950533	11.7981833200
H57	6.2921961374	10.2513242610	13.5092098787
H58	7.5286858556	11.1806738705	12.6313061556
C59	0.8638566875	11.6837252648	11.9611102251
H60	3.1961886089	12.9408903493	10.2689241760
H61	2.1502525946	13.3188065542	11.4778078056
O62	4.1392502115	10.4974084797	8.2034768004
C63	4.3136506213	9.2917478511	7.4861213923
H64	3.3502930436	12.2286457216	9.7909484585
H65	3.4088877652	8.9916682472	6.9110384732
H66	4.5795163298	8.4299697116	8.1389675071
H67	5.1369738305	9.4102559224	6.7569924642

Name – Cis-TS-Dh1\\G=-1721.194248\\H=-1721.098994\\SCF E(PBE-D3/BS1)=-1721.70508684991\\ZeroPoint=358.608

Angstroms

Atom	x	y	z
Fe1	2.1721068579	11.8949289798	10.7857260419
O2	0.1087095114	11.8409242877	12.8136618673
P3	0.7737404237	12.4866473733	9.1305438509
N4	2.0680257806	10.0063146111	9.9458413270
C5	0.7735093967	9.7504196183	9.2938897821
H6	-0.0423119364	9.7194513686	10.0452400708
H7	0.7906718554	8.7622759795	8.7847390590
C8	0.5290827568	10.8551925182	8.2591747771
H9	-0.4501455934	10.7709472345	7.7603295816
H10	1.3297073823	10.7931492254	7.5011138337
P11	3.7442825471	11.0174100879	12.1159676195

C12	1.3168845682	13.7006739747	7.7802470687
H13	0.9892504763	14.6834765553	8.1701767515
C14	2.8386345012	13.7370639564	7.5699933032
H15	3.2485933605	12.7246667095	7.3992617953
H16	3.3523563760	14.1685628068	8.4443620004
H17	3.0769630141	14.3709842904	6.6971046887
C18	0.5851309072	13.4340822530	6.4499445500
H19	0.7815970527	14.2631499176	5.7471809335
H20	-0.5087176084	13.3511946601	6.5648527935
H21	0.9474777587	12.5062827863	5.9762101278
C22	-0.9474773055	13.1596704751	9.4984567047
H23	-1.3258818018	13.5088495276	8.5182760670
C24	-0.8568779814	14.3724599840	10.4413297162
H25	-0.1668343524	15.1461349549	10.0641898359
H26	-0.5076372825	14.0699844338	11.4412178934
H27	-1.8522198675	14.8380353016	10.5518875391
C28	-1.9218684873	12.0961974882	10.0295599035
H29	-2.0524986631	11.2595328799	9.3242615428
H30	-2.9152617463	12.5532988518	10.1861036143
H31	-1.5902457349	11.6856992436	10.9956031912
C32	2.4366541235	8.9394602585	10.8863167466
H33	2.4784367203	7.9604995105	10.3613992912
H34	1.6721189151	8.8478255292	11.6855724276
C35	3.8063225677	9.2571176643	11.4951036371
H36	4.5711046027	9.2315562046	10.6992332859
H37	4.1054702833	8.5348395853	12.2726036433
C38	3.5159773261	10.9095704749	13.9830644811
H39	4.4992298863	10.5764235680	14.3675972841
C40	2.4645276095	9.8735872974	14.4120522675
H41	1.4625822522	10.1290746227	14.0345773564
H42	2.4067553612	9.8447552337	15.5147645891
H43	2.7146547794	8.8561823733	14.0700742366
H44	2.9221748984	10.1487264464	9.0250794087
C45	3.2146412486	12.3023531011	14.5642653778
H46	3.9691822478	13.0519615287	14.2715618611
H47	3.2030329743	12.2538018343	15.6675285140
H48	2.2311283787	12.6665384728	14.2277994867
C49	5.5386503907	11.6256747805	12.0381347130
H50	5.5758382868	12.4222334974	12.8051553659
C51	5.9096670145	12.2456935101	10.6825622037
H52	5.3622398385	13.1842357293	10.5036794406
H53	5.6918096604	11.5640540919	9.8426488038
H54	6.9890971541	12.4770070453	10.6612258217
C55	6.5415683830	10.5223555544	12.4290460965
H56	6.6151343464	9.7523914773	11.6422763593
H57	6.2852060820	10.0168956340	13.3749178667
H58	7.5465823810	10.9630893836	12.5523529265
C59	0.9410977745	11.8123385658	11.9692709350
H60	3.3358764386	12.6645366219	10.0030699368
H61	2.3442136596	13.3144163295	11.3101515609
O62	3.6639672243	10.5609699744	8.0978400912
C63	4.7409543156	9.7200801495	7.8218997093

H64	3.3816286377	11.9256497753	9.5792483415
H65	4.4721382113	8.8311840533	7.1943218346
H66	5.2413398156	9.2993462066	8.7343717963
H67	5.5479577332	10.2534309632	7.2659346743

Name – Cis-TS-Dh2\\G=-1721.185352\\H=-1721.088197\\SCF E(PBE-D3/BS1)=-1721.69542742992\\ZeroPoint=359.008

Angstroms

Atom	x	y	z
Fe1	2.2532216880	11.9382896113	10.7259054203
O2	0.5529389495	12.8611977712	12.8416064189
P3	0.7621106579	12.4847998151	9.1175803940
N4	2.1978530236	10.1650268407	9.9332168348
C5	1.0562205663	9.7662682276	9.0933353689
H6	0.1837812211	9.4851560551	9.7228247025
H7	1.3126507675	8.8571919290	8.5051172072
C8	0.6872079319	10.9003965705	8.1373935158
H9	-0.2946318519	10.7532848467	7.6564484074
H10	1.4565846677	10.9735748738	7.3486116572
P11	3.7493057720	11.0391965851	12.1624175417
C12	1.0646085246	13.8258970927	7.8108651030
H13	0.8591184046	14.7732024983	8.3433030879
C14	2.5247470994	13.8610003426	7.3365124685
H15	2.8669460141	12.8784697721	6.9664022347
H16	3.2042072831	14.1661431099	8.1446433142
H17	2.6274811333	14.5869304635	6.5104239444
C18	0.1063880205	13.7091038369	6.6099883840
H19	0.2927965970	14.5434404256	5.9106020727
H20	-0.9564085601	13.7543500819	6.8955349299
H21	0.2718284222	12.7705304739	6.0537053724
C22	-1.0407711766	12.8105078832	9.5737733628
H23	-1.5712799762	12.8216756685	8.6029486741
C24	-1.2305232341	14.1819645839	10.2449646071
H25	-0.8711431570	15.0123904904	9.6154870266
H26	-0.7063887731	14.2323649540	11.2115446356
H27	-2.3048970360	14.3549386260	10.4344685491
C28	-1.6408616544	11.6724346375	10.4161239758
H29	-1.6239413928	10.7096513251	9.8808837616
H30	-2.6964490697	11.9029875746	10.6470761478
H31	-1.1073485746	11.5470059966	11.3706385419
C32	2.6506367421	8.9993605757	10.7082807855
H33	2.8179383890	8.1312955548	10.0331172744
H34	1.8669332848	8.6761116829	11.4274306013
C35	3.9492122524	9.3290813794	11.4444734256
H36	4.7810752612	9.3803964813	10.7194264502
H37	4.2062187351	8.5806547785	12.2133757049
C38	3.2585575628	10.7140559662	13.9561065621
H39	4.0696192047	10.0718274009	14.3476043356
C40	1.9466944582	9.9199620852	14.0668804790
H41	1.1006968812	10.4659985767	13.6226388409

H42	1.7120770201	9.7443355822	15.1319076850
H43	2.0184921379	8.9350540596	13.5787359513
H44	3.4282789406	10.2656467828	8.6495845164
C45	3.2203389054	12.0049976358	14.7914838866
H46	4.1859375555	12.5372681964	14.7871503774
H47	2.9860556880	11.7569230229	15.8419363637
H48	2.4445347223	12.6971795644	14.4292630175
C49	5.5271480516	11.6663856115	12.3739227388
H50	5.4225656609	12.5590477179	13.0184944813
C51	6.1524207342	12.1179043894	11.0462632224
H52	5.6320944390	12.9924225087	10.6327871072
H53	6.1281648893	11.3216262119	10.2818244093
H54	7.2092418666	12.3922545285	11.2099931532
C55	6.4358403580	10.6427808221	13.0817035807
H56	6.5574590246	9.7279984645	12.4759056849
H57	6.0679070077	10.3478591101	14.0774039693
H58	7.4405228035	11.0802835413	13.2206721358
C59	1.2559847280	12.4678425815	11.9601405914
H60	3.9032809255	12.7210817810	9.4493126742
H61	2.7818803330	13.3645562238	10.8809716804
O62	4.0961446347	10.2555162262	7.8870325881
C63	4.2231137799	8.9122291812	7.4433038553
H64	4.1507648119	12.1296516601	9.0385242013
H65	3.2698820004	8.4925449670	7.0519520443
H66	4.5897653054	8.2240305852	8.2361166129
H67	4.9577654606	8.8867082785	6.6184285157

Name – OFe\\G=-1604.497614\\H=-1604.408226\\SCF E(PBE-D3/BS1)=-1604.94494191930\\ZeroPoint=317.315

Angstroms

Atom	x	y	z
Fe1	1.8707542149	12.0365546566	10.7078885547
O2	2.5805932185	14.8183102890	11.1510032995
P3	0.2822708630	12.4176604549	9.2515126854
N4	2.1031998292	10.4278421461	9.8224022719
C5	1.3370658434	9.9609333203	8.6509234082
H6	0.6348340945	9.1586646760	8.9691112134
H7	2.0252192648	9.4804660593	7.9217363036
C8	0.5669436633	11.0961168474	7.9682916481
H9	-0.3723626348	10.7459107727	7.5064233555
H10	1.1806616403	11.5512450913	7.1726884836
P11	3.3360302358	11.2841145640	12.1359623073
C12	0.2212215138	14.0310754660	8.2818917930
H13	0.0417186761	14.7981898835	9.0591509154
C14	1.5909557808	14.3194566359	7.6435777144
H15	1.8075366731	13.6180474817	6.8187422356
H16	2.4050890354	14.2379036695	8.3806159631
H17	1.6032031657	15.3390356341	7.2197391866
C18	-0.9087022755	14.0927927766	7.2417495319
H19	-0.8712781831	15.0532260890	6.6972741664

H20	-1.9082511764	14.0112200361	7.6985491317
H21	-0.8081301473	13.2861251322	6.4942648951
C22	-1.4881605738	12.1528008460	9.8299528703
H23	-2.1303888600	12.1723333592	8.9286785251
C24	-1.9111044654	13.2759490299	10.7885381532
H25	-1.9068820108	14.2662035459	10.3027356536
H26	-1.2250209438	13.3167340478	11.6527740626
H27	-2.9324980231	13.0922759973	11.1667204631
C28	-1.6036442018	10.7738702386	10.4996029015
H29	-1.4097911216	9.9518520704	9.7907963337
H30	-2.6198588173	10.6306181607	10.9087460808
H31	-0.8744639286	10.6916462460	11.3239549337
C32	3.0122107066	9.3368013293	10.2318535142
H33	3.8800102014	9.3097998764	9.5379142919
H34	2.5029517093	8.3560283593	10.1129679931
C35	3.4929871793	9.4851644880	11.6808512489
H36	4.5178392079	9.1019562204	11.8254017505
H37	2.8325098034	8.9225913125	12.3612805729
C38	2.9810203895	11.3061261881	13.9819437006
H39	3.7916636540	10.7342934885	14.4734212027
C40	1.6338419814	10.6314473454	14.2853800770
H41	0.8213697787	11.1431606750	13.7418580060
H42	1.4211302918	10.6828760047	15.3680932670
H43	1.6160999232	9.5686080693	13.9923339645
H44	0.8899058649	12.2255410450	11.8133816550
C45	2.9916894026	12.7580232157	14.4902228827
H46	3.9722538671	13.2446976741	14.3577465159
H47	2.7448516075	12.7885252775	15.5661012572
H48	2.2390214492	13.3571329010	13.9492392379
C49	5.0736101616	11.9959656465	11.9772911672
H50	4.9356721237	13.0736245665	12.1868353396
C51	5.5307147130	11.8547045497	10.5147556026
H52	4.7555031545	12.2285014879	9.8246585871
H53	5.7334523332	10.7997191943	10.2593822608
H54	6.4628134276	12.4219472595	10.3456737068
C55	6.1039542613	11.4197514084	12.9586489560
H56	6.2195787167	10.3290625322	12.8296564704
H57	5.8366575873	11.6102797219	14.0107005296
H58	7.0938881432	11.8766626049	12.7800650255
C59	2.2708722246	13.6782963363	10.9772332595

Natural Bond order analysis data

Table S2: Population analysis data along IRC in TS-A1.

	1Fe	2N	3CO	4H	5P	6P	7Me	8Me	9H	10Me	11O
1	26.31669	7.67537	13.93949	1.09132	13.83315	13.86484	66.55711	66.57474	0.52953	8.79799	8.81974
2	26.31831	7.67962	13.93931	1.08892	13.83244	13.86594	66.55737	66.57452	0.52749	8.79603	8.82006
3	26.31991	7.68374	13.93942	1.08594	13.83141	13.86754	66.55755	66.57435	0.52626	8.79366	8.82022
4	26.32216	7.68707	13.9394	1.08288	13.83039	13.86867	66.55811	66.57413	0.52607	8.79075	8.82038
5	26.32509	7.68974	13.93962	1.07896	13.82954	13.87	66.55865	66.5742	0.52676	8.78723	8.8202
6	26.32149	7.69193	13.94112	1.07674	13.82899	13.87417	66.55675	66.57342	0.52818	8.78344	8.82018
7	26.32361	7.69407	13.94248	1.07265	13.82825	13.87569	66.56167	66.57377	0.52995	8.77869	8.81919
8	26.32623	7.69568	13.94419	1.06782	13.82741	13.87716	66.56343	66.57475	0.53172	8.77374	8.81788
9	26.3285	7.69762	13.9461	1.06306	13.82693	13.87846	66.5653	66.57581	0.53311	8.76877	8.81635
10	26.33085	7.69947	13.94816	1.05824	13.82682	13.88003	66.56754	66.57745	0.53385	8.7636	8.81401
11	26.33362	7.70149	13.95038	1.05335	13.82671	13.88128	66.5701	66.57939	0.53363	8.75844	8.81156
12	26.33582	7.70354	13.95261	1.04878	13.82686	13.88253	66.57472	66.58152	0.53271	8.75357	8.80936
13	26.34068	7.70579	13.95514	1.0424	13.82774	13.88454	66.57501	66.58641	0.53031	8.74801	8.80669
14	26.34275	7.7086	13.95749	1.0385	13.82684	13.88479	66.57755	66.58627	0.52832	8.74373	8.80515
15	26.34482	7.71042	13.98018	1.03475	13.82691	13.88523	66.58009	66.58887	0.52605	8.7398	8.80287
16	26.34785	7.71166	13.96218	1.031	13.82679	13.88542	66.58287	66.59158	0.52359	8.73665	8.80039
17	26.348	7.71314	13.96492	1.02782	13.82698	13.88636	66.58526	66.59376	0.52108	8.73349	8.79917
18	26.34882	7.71417	13.96792	1.02489	13.82713	13.88651	66.58782	66.59667	0.51824	8.73067	8.79714
19	26.34912	7.71493	13.97025	1.02241	13.82743	13.88657	66.59013	66.5993	0.5158	8.72856	8.79551
20	26.35125	7.7155	13.97175	1.01951	13.82799	13.88702	66.59218	66.60168	0.51309	8.72638	8.7937
21	26.35182	7.71598	13.97325	1.01776	13.82808	13.88799	66.59448	66.60423	0.51063	8.72444	8.7922
22	26.35341	7.71646	13.97422	1.01562	13.82861	13.88711	66.59656	66.60648	0.50823	8.72264	8.79066
23	26.35468	7.71687	13.97495	1.01389	13.82884	13.88688	66.59885	66.61068	0.506	8.72093	8.78941

Table S3: Population analysis data along IRC in TS-B1.

	1Fe	2N	3CO	4H	5P	6P	7H	8H	9O	10CH2	11Me	12Me
1	26.38806	7.69	13.9657	0.97133	13.86743	13.872	0.86534	0.54168	8.7982	7.94196	66.54112	66.53711
2	26.42605	7.68736	13.9632	0.98048	13.86502	13.86886	0.89107	0.54201	8.7894	7.88194	66.54506	66.53911
3	26.44145	7.68353	13.95968	0.98859	13.86222	13.86695	0.92942	0.5424	8.77616	7.85551	66.5509	66.54001
4	26.46281	7.67824	13.95492	1.00609	13.85831	13.86247	0.95828	0.5426	8.75846	7.82394	66.55152	66.54172
5	26.47213	7.67537	13.95279	1.02238	13.85736	13.86031	0.98588	0.54301	8.74159	7.79049	66.55448	66.54421
6	26.48309	7.67259	13.95056	1.03615	13.85604	13.85727	1.01239	0.54345	8.72433	7.75919	66.55802	66.54695
7	26.49312	7.66981	13.94909	1.04868	13.85469	13.85474	1.03817	0.54396	8.70772	7.72842	66.56174	66.54985
8	26.50318	7.66721	13.94823	1.06126	13.84984	13.85334	1.06199	0.5447	8.69086	7.69879	66.5679	66.55267
9	26.51197	7.66452	13.94778	1.07315	13.84906	13.8507	1.08248	0.54556	8.67573	7.67135	66.57188	66.55621
10	26.51949	7.66225	13.94752	1.08366	13.84781	13.84934	1.10035	0.54648	8.66103	7.6471	66.57559	66.55845
11	26.52446	7.66089	13.94711	1.09378	13.84742	13.84882	1.11521	0.54739	8.64822	7.62541	66.57895	66.56234
12	26.52946	7.65836	13.94742	1.10368	13.84669	13.84744	1.12831	0.54849	8.63577	7.60598	66.58271	66.56568
13	26.53447	7.65672	13.94782	1.11174	13.84608	13.84661	1.13911	0.54917	8.63512	7.58881	66.58572	66.5686
14	26.53795	7.65557	13.94863	1.1187	13.8452	13.84641	1.14838	0.54963	8.61587	7.57369	66.58853	66.57143
15	26.54041	7.65558	13.9491	1.12517	13.84504	13.84733	1.1553	0.5499	8.60809	7.56023	66.59042	66.57345
16	26.54293	7.65381	13.95021	1.13123	13.84583	13.84702	1.16245	0.55036	8.60015	7.54864	66.59043	66.57654
17	26.53963	7.65302	13.95149	1.13808	13.84714	13.84714	1.16864	0.55075	8.59335	7.52873	66.59377	66.5788
18	26.54107	7.65221	13.95237	1.14318	13.84679	13.84702	1.17347	0.55096	8.58715	7.52958	66.59536	66.58082
19	26.54249	7.65169	13.95304	1.14772	13.84682	13.84708	1.17708	0.55154	8.58136	7.52166	66.59727	66.58256
20	26.5441	7.65094	13.95378	1.15206	13.84673	13.84683	1.18024	0.55154	8.57568	7.51496	66.59889	66.58453
21	26.54462	7.65043	13.9545	1.1566	13.84664	13.84682	1.18275	0.55184	8.57049	7.50886	66.60046	66.58604