Is Aromaticity Loss Necessary for Transition-Metal Promoted Arene-Alkene Cycloadditions?

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1. Computed activation free energies for *endo* vs. *exo* reactions

Table S1. Computed activation free energies (kcal/mol) for *endo* and *exo* pathways at ωB97X-D/def2-TZVPP//ωB97X-D/def2-SVP.

Reactants	Product	$\Delta G^{‡}$	ΔG_{prod}
Benzene + cyclopentadiene	*endo*	48.3	21.0
	exo	46.8	20.2
p-nitroaniline + cyclopentadiene	*endo*	41.0	13.4
	exo	41.1	14.3
1 + NMN	*endo*	25.2	−14.3
	exo	22.9	–14.9
2 + NMN	*endo*	26.3	–11.7
	exo	23.3	–13.6
3 + NMN	*endo*	32.8	–8.2
	exo	--[a]	--[a]
Benzene + NMN	–	38.3	9.5
7' + NMN	*endo*	13.4	–36.3
	exo	10.6	–38.4
16 + NMN	*endo*	31.0	-8.2
	exo	31.3	-6.6
14 + bis(trifluoromethyl)tetrazine	–	14.7	–25.9
14 + cyclopentadiene	*endo*	29.2	–16.9
	exo	32.6	–17.8
11 + cyclopentadiene	*endo*	27.7	–15.4
	exo	31.4	–15.3
11 + bis(trifluoromethyl)tetrazine	–	15.3	–20.9
11 + Danishefsky diene	*endo*	31.4	–21.0
	exo	32.4	–24.7

[a] Geometry optimization did not lead to a sigma complex.

Table S2. Computed activation free energies (kcal/mol) for *endo* and *exo* pathways at DLPNO-CCSD(T)/def2-TZVPP//ωB97X-D/def2-SVP.

Reactants	Product	$\Delta G^{\ddagger}$	ΔG_{prod}
Benzene + cyclopentadiene	*endo*	44.0	17.2
	exo	42.4	16.4
p-nitroaniline + cyclopentadiene	*endo*	37.8	11.1
	exo	37.2	12.0
1 + NMN	*endo*	21.7	–15.4
	exo	19.7	–15.5
2 + NMN	*endo*	23.1	–12.4
	exo	23.4	–10.6
3 + NMN	*endo*	25.4	–7.7
	exo	--[a]	--[a]
Benzene + NMN	–	34.0	6.1
7' + NMN	*endo*	10.5	–35.8
	exo	7.5	–37.3
16 + NMN	*endo*	27.0	–9.9
	exo	27.9	–9.8
14 + bis(trifluoromethyl)tetrazine	–	11.1	–30.6
14 + cyclopentadiene	*endo*	26.2	–18.1
	exo	29.2	–19.1
11 + cyclopentadiene	*endo*	24.8	–17.8
	exo	28.7	–18.1
11 + bis(trifluoromethyl)tetrazine	–	11.2	–26.7
11 + Danishefsky diene	*endo*	29.5	–22.0
	exo	30.6	–26.1

[a] Geometry optimization did not lead to a sigma complex.

2. Benchmark studies

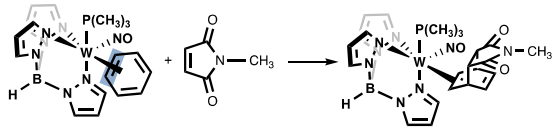

Figure S1. Reaction selected for benchmark study (cf. Figure 3c in main text).

Gibbs free energies were computed based on the sum of total electronic energy of the selected functional with a def2-TZVPP basis set and free energy correction terms at the ωB97X-D/def2-SVP level. All structures were optimized at the ωB97X-D/def2-SVP level. Single-point energies calculated at the ωB97X-D, PW6B95, M06, M06-L, MN15, and PBE0-D3/def2-TZVPP levels were benchmarked against results at the DLPNO-CCSD(T)/def2-TZVPP level. Computed free energy barriers ($\Delta G^{\ddagger}$) for all functionals are all within ca. ±3 kcal/mol compared to data computed at DLPNO-CCSD(T)/def2-TZVPP (19.7 kcal/mol). Computed relative free energies (ΔG) for ωB97X-D, MN15, and PBE0-D3 are within ca. ±1 kcal/mol compared to data computed at DLPNO-CCSD(T)/def2-TZVPP (–15.5 kcal/mol); PW6B95, M06, M06-L gave large discrepancies. Since results at the ωB97X-D/def2-TZVPP level are in close agreement with DLPNO-CCSD(T)/def2-TZVPP data, the ωB97X-D functional was selected for the study here.

Table S3. Activation free energy barriers ($\Delta G^{\ddagger}$) and relative free energies between the σ-complex and product (ΔG) computed with selected functionals with the def2-TZVPP basis set and benchmarked against results at the DLPNO-CCSD(T)/def2-TZVPP level. All structures were optimized at the ωB97X-D/def2-SVP level.

Level of Theory	$\Delta G^{\ddagger}$, kcal mol^{-1}	ΔG, kcal mol^{-1}
ωB97X-D	22.9	−14.9
PW6B95	21.0	−9.1
M06	23.1	−9.7
M06-L	24.4	−1.7
MN15	21.3	−12.4
PBE0-D3	16.8	−16.3
DLPNO-CCSD(T)	**19.7**	**−15.5**

3. Additional schemes

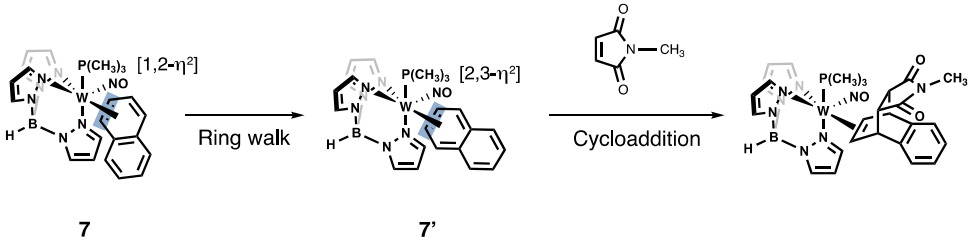

Figure S2. Diels–Alder reaction of **7** with NMM.

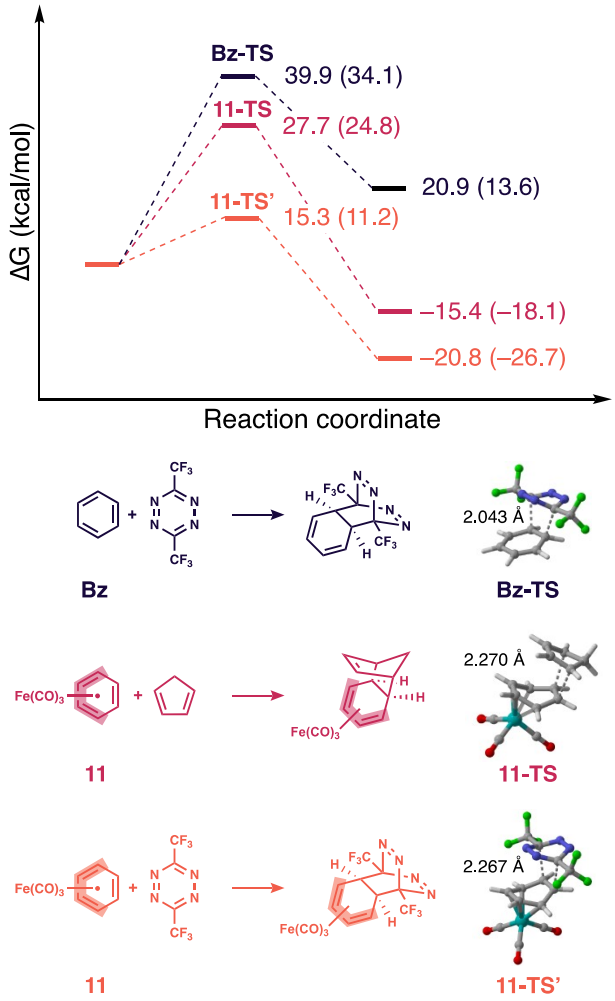

Figure S3. Computed reaction profiles for Diels–Alder reactions for benzene with bis(trifluoromethyl)tetrazine, **11** with cyclopentadiene, and **11** with bis(trifluoromethyl)tetrazine at *ω*B97X-D/def2-TZVPP//*ω*B97X-D/def2-SVP. Single-point energies at DLPNO-CCSD(T)/def2-TZVPP//*ω*B97X-D/def2-SVP are shown in parenthesis. All reaction barriers are computed relative to a σ-complex of the reactants.

Table S4. Computed HOMA values for relevant compounds.

Compound	rHOMA
Benzene	1.0
Naphthalene	0.782
Aniline	0.969
Nitrobenzene	0.992
p-Nitroaniline	0.950
1	0.139
2	0.286
3	0.632
4	0.064
5	0.363
6	0.800
7	Ring A: –0.042 Ring B: 0.941
7’	Ring A: 0.282 Ring B: 0.303
8	Ring A: 0.061 Ring B: 0.936
8’	Ring A: 0.434 Ring B: 0.379
9	–0.350
10	–0.297
11	–0.124
12	0.059
13	–0.181
14	–0.509
15	0.844
16	Ring A: 0.636 Ring B: 0.699

4. Optimized Cartesian coordinates for arenes and complexed arenes

Benzene

C	2.17834	-2.52135	-0.14102
C	3.57336	-2.52140	-0.14045
C	4.27086	-1.31349	-0.14120
C	3.57340	-0.10533	-0.14210
C	2.17859	-0.10528	-0.14249
C	1.48099	-1.31336	-0.14210
H	1.63238	-3.46707	-0.14065
H	4.11923	-3.46719	-0.13972
H	5.36285	-1.31339	-0.14095
H	4.11959	0.84025	-0.14256
H	1.63252	0.84038	-0.14331
H	0.38898	-1.31320	-0.14245

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –232.0014242
Number of imaginary frequencies: 0

Naphthalene

C	-3.91613	-0.81590	0.00033
C	-2.54302	-0.81391	0.00014
C	-1.81624	0.40869	0.00024
C	-2.53662	1.63898	0.00052
C	-3.95849	1.60343	0.00069
C	-4.63216	0.40694	0.00061
H	0.15568	-0.50029	-0.00016
H	-4.46243	-1.76162	0.00027
H	-1.98848	-1.75580	-0.00007
C	-0.39436	0.44424	0.00006
C	-1.80984	2.86159	0.00060
H	-4.50854	2.54796	0.00091
H	-5.72424	0.39331	0.00075
C	-0.43673	2.86357	0.00042
C	0.27929	1.64073	0.00016
H	-2.36439	3.80348	0.00081
H	0.10958	3.80929	0.00049
H	1.37138	1.65438	0.00001

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –385.4832425
Number of imaginary frequencies: 0

Indole

C	0.82181	-0.03127	0.06505
C	-0.55792	-0.35225	0.00713
C	-1.54527	0.62669	-0.16509
C	-1.12854	1.94372	-0.27966

C	0.23887	2.28560	-0.22483
C	1.21236	1.31450	-0.05432
C	1.52921	-1.27006	0.24658
C	0.58616	-2.26026	0.29039
H	-2.60441	0.36332	-0.20770
H	-1.87276	2.73163	-0.41490
H	0.53021	3.33393	-0.31872
H	2.26926	1.58753	-0.01287
H	2.60441	-1.40535	0.33343
H	-1.53378	-2.23329	0.14500
N	-0.66855	-1.71473	0.14715
H	0.71074	-3.33393	0.41490

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –363.4394936
Number of imaginary frequencies: 0

Aniline

C	2.82260	0.00000	0.00000
C	2.11246	1.20040	0.00019
C	0.72094	1.20635	0.00017
C	0.00000	0.00000	0.00000
C	0.72098	-1.20635	-0.00006
C	2.11251	-1.20040	0.00000
H	3.91398	0.00016	-0.00073
H	2.64906	2.15228	-0.00049
H	0.17866	2.15578	0.00422
H	0.17873	-2.15580	0.00397
H	2.64892	-2.15238	-0.00099
N	-1.38504	-0.00011	0.04686
H	-1.84388	0.84311	-0.27154
H	-1.84358	-0.84370	-0.27103

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –287.614645512
Number of imaginary frequencies: 0

Nitrobenzene

C	2.51021	-0.00001	0.00007
C	1.81626	1.18282	-0.25844
C	0.42409	1.19087	-0.26016
C	-0.24587	-0.00009	-0.00006
C	0.42414	-1.19102	0.26011
C	1.81631	-1.18288	0.25851
H	3.60214	0.00001	0.00011
H	2.36201	2.10628	-0.46032
H	-0.14987	2.09556	-0.45779
H	-0.14980	-2.09572	0.45772

H	2.36212	-2.10629	0.46044
N	-1.72190	-0.00002	-0.00011
O	-2.28102	1.04988	-0.22789
O	-2.28135	-1.04973	0.22782

Electronic energy (a.u.) at ωB97X-D/def2-SVP: −436.2831699
Number of imaginary frequencies: 0

p-nitroaniline

C	-2.07511	0.06258	-0.00682
C	-1.37654	-1.13744	0.24399
C	0.00760	-1.16413	0.24587
C	0.71694	0.00948	-0.00306
C	0.05334	1.20922	-0.25360
C	-1.33084	1.23525	-0.25532
H	-1.93564	-2.05589	0.43669
H	0.55567	-2.08586	0.43941
H	0.63707	2.10957	-0.44375
H	-1.85411	2.17341	-0.45360
N	2.17735	-0.01763	0.00043
O	2.76226	1.02344	-0.21847
O	2.72233	-1.07957	0.22203
N	-3.44153	0.08229	-0.03807
H	-3.95519	-0.70760	0.32358
H	-3.92299	0.96925	-0.02865

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –491.59024
Number of imaginary frequencies: 0

Compound 1

W	-0.35181	0.16710	-0.10348
P	-1.51694	-2.05336	-0.14939
O	-1.82539	0.90390	-2.55797
N	0.90686	-0.55180	1.71717
N	2.24780	-0.57353	1.63781
N	1.28067	-0.83083	-1.28279
N	2.55185	-0.89857	-0.85272
N	1.30317	1.70653	-0.20716
N	2.57794	1.38872	0.08761
N	-1.22928	0.63558	-1.55903
C	-2.08456	0.53899	1.32738
C	-1.22897	1.72013	1.23402
C	-1.79520	2.92851	0.65111
C	-3.02527	2.93911	0.07894
C	-3.86618	1.76937	0.15147
C	-3.44004	0.65717	0.80079

C	2.77433	-1.01897	2.79102
C	1.73586	-1.30142	3.66506
C	0.58290	-0.98538	2.93667
C	3.32290	-1.47395	-1.79298
C	2.52291	-1.79704	-2.87819
C	1.24603	-1.35557	-2.50717
C	3.37507	2.45365	-0.12324
C	2.59199	3.50322	-0.57291
C	1.29401	2.97367	-0.61276
C	-2.87474	-2.09870	-1.37139
C	-2.30523	-2.72489	1.36875
C	-0.47865	-3.49809	-0.61701
B	2.98640	-0.07143	0.38092
H	-1.99592	-0.08389	2.22532
H	4.18487	-0.15599	0.54498
H	-0.49269	1.87954	2.03178
H	-1.21099	3.85116	0.70347
H	-3.41489	3.85058	-0.37929
H	-4.87835	1.81235	-0.25688
H	-4.13670	-0.17378	0.95348
H	3.85179	-1.09943	2.91109
H	1.80298	-1.67453	4.68254
H	-0.45943	-1.03955	3.24175
H	4.39062	-1.59868	-1.63029
H	2.82233	-2.26917	-3.80901
H	0.31039	-1.37133	-3.06318
H	4.44520	2.38505	0.05605
H	2.91181	4.50620	-0.83893
H	0.35826	3.43394	-0.92024
H	-3.60561	-1.32046	-1.11155
H	-2.47307	-1.83936	-2.36094
H	-3.36318	-3.08346	-1.40807
H	-1.54144	-2.85499	2.14872
H	-3.07517	-2.03761	1.74153
H	-2.76747	-3.70145	1.16175
H	0.39014	-3.54492	0.05643
H	-0.10223	-3.38389	-1.64115
H	-1.04775	-4.43682	-0.54562

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1591.61003619
Number of imaginary frequencies: 0

Compound 2

Re	-0.93948	-0.73959	-0.47680
C	-1.04947	-2.95306	-0.35982
C	-1.13816	-2.55067	-1.75190

C	-2.38007	-2.82077	-2.45522
C	-3.47159	-3.32044	-1.81645
C	-3.39126	-3.69458	-0.43014
C	-2.21968	-3.56468	0.24720
N	-0.92911	0.21731	-2.43401
C	-1.83566	0.27384	-3.40635
C	-1.38040	1.10118	-4.44391
C	-0.14318	1.54446	-4.01053
N	0.10408	0.99838	-2.80344
N	1.31659	-0.96460	-0.80562
C	2.20653	-1.93046	-0.57469
C	3.47552	-1.54536	-1.03127
C	3.27476	-0.27852	-1.55634
N	1.97651	0.03876	-1.40576
N	-0.38291	1.29883	0.09078
C	-0.80359	2.08644	1.07970
C	-0.07793	3.28628	1.07868
C	0.79511	3.15700	0.00911
N	0.59261	1.95466	-0.55874
B	1.24054	1.33192	-1.81867
N	-0.65316	-1.06187	1.65886
C	-1.61443	-1.34173	2.59878
C	-1.03891	-1.34025	3.83991
N	0.29218	-1.05326	3.64640
C	0.47725	-0.89254	2.31790
C	1.30437	-0.93189	4.67252
C	-2.76394	-0.47326	-0.25640
O	-3.91213	-0.29740	-0.10540
H	-0.09115	-3.31045	0.03420
H	-0.23019	-2.57766	-2.36529
H	-2.41633	-2.63769	-3.53256
H	-4.40104	-3.49171	-2.36424
H	-4.26441	-4.13416	0.05759
H	-2.13571	-3.94290	1.27025
H	-2.76816	-0.27536	-3.30346
H	-1.88727	1.34558	-5.37263
H	0.57793	2.21651	-4.46900
H	1.89850	-2.85892	-0.09882
H	4.40104	-2.11225	-0.99292
H	3.96280	0.41825	-2.02875
H	-1.60928	1.75229	1.73012
H	-0.18797	4.13416	1.74829
H	1.53909	3.83946	-0.39435
H	2.02411	2.11195	-2.31899
H	-2.64686	-1.51845	2.30922
H	-1.45522	-1.51301	4.82827

H	1.43531	-0.64320	1.86651
H	2.26613	-0.69698	4.20080
H	1.40532	-1.87415	5.22892
H	1.04928	-0.12414	5.37263

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1390.6046139
Number of imaginary frequencies: 0

Compound 3

Os	0.21103	0.55629	-0.12066
N	-0.36540	2.67926	-0.16376
H	-0.68793	3.05831	0.73149
H	0.40628	3.29856	-0.43364
N	-1.91114	-0.02715	0.01092
H	-2.42618	0.03962	-0.87182
H	-2.07012	-0.98955	0.32527
N	-0.02002	0.41858	-2.30326
H	0.03593	1.31485	-2.79588
H	0.72777	-0.14469	-2.72010
N	0.15753	0.53258	2.07442
H	0.93384	-0.01731	2.45671
H	0.26306	1.45005	2.51780
N	0.78256	-1.54734	-0.09370
H	1.75701	-1.64914	-0.40273
H	0.75734	-2.00007	0.82396
C	2.32265	1.31735	0.48025
C	3.14894	0.39034	1.21072
C	3.84777	-0.59020	0.56057
C	3.81238	-0.67468	-0.86595
C	3.07852	0.22552	-1.59232
C	2.28554	1.23140	-0.93479
H	2.10307	2.27067	0.97157
H	3.28168	0.52526	2.28777
H	4.49564	-1.26716	1.12147
H	4.43690	-1.41169	-1.37573
H	3.15338	0.22991	-2.68323
H	2.03553	2.11814	-1.52631
H	-1.11739	2.91032	-0.81954
H	-0.88746	-0.00914	-2.63979
H	-2.45664	0.55199	0.65648
H	-0.68541	0.13326	2.49700
H	0.24308	-2.16721	-0.70421

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –604.8462931
Number of imaginary frequencies: 0

Compound 4

Cr	-0.62345	0.12094	-0.03072
C	0.16151	-0.84517	-1.33353
C	-2.22355	-0.73730	-0.44056
C	0.97606	1.02084	0.17862
C	-1.26922	1.58906	-0.85199
O	1.99262	1.61063	0.22263
O	-3.21236	-1.24601	-0.80080
O	0.67603	-1.45668	-2.20532
O	-1.67683	2.54679	-1.41357
C	-2.33444	-2.24419	2.49870
C	-1.03022	-2.18843	2.10397
C	-0.32485	-0.95005	1.84393
C	-1.06580	0.31006	2.09513
C	-2.42623	0.18580	2.57732
C	-3.06009	-1.01007	2.74476
H	-2.83726	-3.20949	2.63332
H	-0.47291	-3.12700	1.97300
H	0.74927	-0.98649	2.06252
H	-0.52171	1.17502	2.49347
H	-2.96584	1.11284	2.81832
H	-4.10852	-1.04743	3.06438

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-1729.1258583
Number of imaginary frequencies: 0

Compound 5

Mn	-0.63121	0.12031	-0.05302
C	0.15595	-0.91464	-1.26477
C	-2.20661	-0.74006	-0.38459
C	0.93994	0.99476	0.19718
C	-1.32035	1.59546	-0.76582
O	1.94169	1.55648	0.33589
O	-3.19554	-1.26892	-0.64972
O	0.66675	-1.56543	-2.08232
O	-1.75491	2.55251	-1.26387
C	-2.31852	-2.21390	2.43253
C	-1.01336	-2.17133	2.04494
C	-0.32013	-0.92134	1.81657
C	-1.04371	0.30942	2.06164
C	-2.41342	0.21012	2.51898
C	-3.03795	-0.99019	2.67614
H	-2.82157	-3.17404	2.57703
H	-0.45585	-3.10313	1.90471
H	0.76099	-0.95152	1.97644
H	-0.50071	1.19455	2.40367

H	-2.94873	1.13717	2.74870
H	-4.08054	-1.03262	3.00327

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1835.7735574
Number of imaginary frequencies: 0

Compound 6

Fe	-0.62533	0.13551	-0.11238
C	0.18734	-0.99624	-1.22185
C	-2.19306	-0.72344	-0.42904
C	0.94167	1.01299	0.11073
C	-1.36667	1.64592	-0.69655
O	1.92971	1.56732	0.24636
O	-3.17416	-1.25534	-0.65535
O	0.68945	-1.66805	-2.00391
O	-1.81772	2.59465	-1.15649
C	-2.33211	-2.20410	2.40854
C	-1.00262	-2.16872	2.06450
C	-0.32173	-0.92354	1.93321
C	-1.02662	0.27552	2.17202
C	-2.40247	0.21253	2.53854
C	-3.04051	-0.99908	2.64839
H	-2.84512	-3.16215	2.51343
H	-0.44705	-3.09551	1.90717
H	0.76893	-0.93314	1.92687
H	-0.48938	1.20734	2.35305
H	-2.93733	1.14064	2.75043
H	-4.09301	-1.03944	2.93590

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1948.4356211
Number of imaginary frequencies: 0

Compound 7

W	0.43633	0.17188	-0.52891
P	2.70254	-0.44557	0.38472
O	0.95289	2.99446	0.17883
N	-1.80330	0.29835	-0.65447
N	-2.59351	-0.69934	-0.20841
N	0.02654	-2.08114	-0.90370
N	-1.02463	-2.67888	-0.31952
N	-0.30405	-0.32092	1.54308
N	-1.22822	-1.26917	1.77044
N	0.72644	1.86415	-0.12646
C	2.15342	2.57231	-2.94085
H	2.85001	3.41102	-3.01329
C	2.59097	1.35024	-2.57500

H	3.65952	1.20382	-2.38534
C	1.68732	0.20836	-2.40624
C	0.28414	0.42136	-2.72982
C	0.33724	4.03349	-3.83287
H	1.03586	4.87461	-3.83219
C	-1.40832	1.87281	-3.87418
H	-2.09223	1.02016	-3.89636
C	0.77028	2.79382	-3.33882
C	-0.13217	1.70277	-3.31607
C	-0.94818	4.19796	-4.33454
C	-1.81876	3.10483	-4.37201
C	-3.88581	-0.32833	-0.29930
H	-4.67558	-1.00179	0.02459
C	-3.93879	0.95226	-0.82115
H	-4.81991	1.55211	-1.02768
C	-2.59469	1.30411	-1.01705
H	-2.16251	2.22439	-1.40145
C	-1.08550	-3.97064	-0.68427
H	-1.87842	-4.61329	-0.30983
C	-0.03012	-4.23178	-1.54490
H	0.21726	-5.17061	-2.03105
C	0.63520	-3.00463	-1.64990
H	1.51126	-2.74378	-2.23926
C	-1.53802	-1.30065	3.07870
H	-2.28647	-1.99538	3.45184
C	-0.78377	-0.33739	3.73171
H	-0.78883	-0.09182	4.78937
C	-0.03333	0.26059	2.71112
H	0.67374	1.08699	2.75456
C	3.67025	1.01816	0.89620
H	4.65179	0.74066	1.30770
H	3.09773	1.58457	1.64386
H	3.79544	1.67620	0.02493
C	3.89698	-1.38642	-0.64497
H	4.14749	-0.82878	-1.55610
H	3.45025	-2.34850	-0.93353
H	4.81991	-1.58133	-0.07904
C	2.68892	-1.50621	1.88628
H	2.11058	-2.41647	1.66808
H	2.19683	-0.98876	2.71915
H	3.70988	-1.78524	2.18581
B	-1.99931	-1.88863	0.57606
H	-2.87799	-2.62162	0.97697
H	2.12636	-0.76401	-2.65997
H	-0.27256	-0.44520	-3.10803
H	-1.26846	5.17061	-4.71456

H	-2.82242	3.21658	-4.78937

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1745.1106979
Number of imaginary frequencies: 0

Compound 7'

W	0.43658	-0.06549	-0.67328
P	2.89512	-0.30829	-0.25966
O	0.74818	2.85165	-0.30511
N	-1.80498	-0.19793	-0.40628
N	-2.37101	-1.20384	0.28690
N	0.22382	-2.37877	-0.78489
N	-0.62526	-3.01130	0.04217
N	0.15503	-0.41694	1.51928
N	-0.60322	-1.41588	2.00323
N	0.60117	1.67897	-0.46937
C	2.00443	1.00690	-3.31233
H	3.08614	0.90663	-3.45127
C	1.25633	-0.12314	-2.82298
C	-0.20579	-0.01553	-2.82939
C	-0.79312	1.19452	-3.33720
C	2.17737	3.35981	-4.04724
H	3.26876	3.28865	-4.03524
C	-0.63718	3.54576	-4.08420
H	-1.72825	3.61779	-4.09927
C	1.41284	2.20446	-3.63539
C	-0.04240	2.30190	-3.65423
C	1.56671	4.50907	-4.43211
C	0.12826	4.60488	-4.45141
C	-3.69997	-1.00415	0.37971
H	-4.32805	-1.71349	0.91299
C	-4.01119	0.17512	-0.27550
H	-4.98836	0.63403	-0.39218
C	-2.77643	0.64536	-0.74625
H	-2.53585	1.54962	-1.29998
C	-0.59702	-4.33497	-0.18600
H	-1.22593	-5.00812	0.39127
C	0.30811	-4.58322	-1.20653
H	0.57405	-5.54061	-1.64423
C	0.79267	-3.31497	-1.54691
H	1.51466	-3.03876	-2.31166
C	-0.66700	-1.33279	3.34463
H	-1.25272	-2.05008	3.91424
C	0.07988	-0.23843	3.75220
H	0.23890	0.11945	4.76492
C	0.56455	0.31088	2.55799

H	1.16911	1.20048	2.39136
C	3.75480	1.30470	-0.26447
H	4.83006	1.19947	-0.05854
H	3.28894	1.95940	0.48535
H	3.59962	1.78280	-1.24173
C	3.94004	-1.33434	-1.37193
H	3.88901	-0.96432	-2.40385
H	3.58256	-2.37392	-1.35171
H	4.98836	-1.31647	-1.03890
C	3.37457	-1.03679	1.35990
H	2.88542	-2.01618	1.46934
H	3.03181	-0.39794	2.18326
H	4.46505	-1.16231	1.43295
B	-1.50188	-2.23212	1.04308
H	-2.19792	-3.00280	1.66905
H	-0.78915	-0.93274	-2.97174
H	-1.87467	1.22495	-3.49551
H	2.16248	5.37412	-4.73223
H	-0.33991	5.54061	-4.76492
H	1.69901	-1.10289	-3.03241

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1745.0793217
Number of imaginary frequencies: 0

Compound 8

Re	-0.31356	-0.02665	-0.65034
N	-0.06557	1.13743	-2.47927
C	-0.86595	1.33775	-3.52360
C	-0.27853	2.24704	-4.41505
C	0.92310	2.58479	-3.81686
N	1.02664	1.90413	-2.65891
N	1.95747	-0.31315	-0.78422
C	2.78680	-1.33865	-0.58492
C	4.10751	-0.96245	-0.86883
C	4.00385	0.36345	-1.25818
N	2.70874	0.72052	-1.19623
N	0.24742	1.93184	0.18147
C	-0.25148	2.63679	1.19575
C	0.51178	3.79570	1.39543
C	1.49227	3.73195	0.41685
N	1.31125	2.60219	-0.28968
B	2.06621	2.08226	-1.53564
N	-0.27395	-0.53644	1.46409
C	-1.35282	-0.72383	2.29293
C	-0.90654	-0.88156	3.57586
N	0.46507	-0.79240	3.51993

C	0.80055	-0.58281	2.22960
C	1.37852	-0.88470	4.63778
C	-2.14030	0.30235	-0.58773
O	-3.28845	0.52440	-0.53912
H	-1.82393	0.82649	-3.57278
H	-0.67900	2.61037	-5.35669
H	1.71034	3.26760	-4.12643
H	2.40251	-2.30081	-0.25384
H	5.00434	-1.57190	-0.80872
H	4.75917	1.07713	-1.57782
H	-1.13393	2.27789	1.72142
H	0.35910	4.57716	2.13388
H	2.29989	4.41563	0.16704
H	2.92424	2.87256	-1.86945
H	-2.36734	-0.74335	1.90485
H	-1.43794	-1.05650	4.50674
H	1.82382	-0.45206	1.88412
H	2.40746	-0.79741	4.26853
H	1.26729	-1.85226	5.14648
H	1.19191	-0.07473	5.35669
C	-2.90089	-4.08359	1.46204
C	-1.73249	-3.51914	0.96608
C	-1.70800	-2.86484	-0.27583
C	-2.88816	-2.84681	-1.05918
C	-4.06387	-3.41286	-0.53887
C	-4.07979	-4.01629	0.71143
H	-2.89874	-4.57716	2.43709
H	-0.81121	-3.56520	1.55400
C	-0.48807	-2.21428	-0.76998
C	-2.83173	-2.30952	-2.40894
H	-4.97511	-3.38157	-1.14235
H	-5.00434	-4.45035	1.09885
C	-1.68543	-1.80500	-2.91391
C	-0.47210	-1.66998	-2.10994
H	-3.73340	-2.36717	-3.02371
H	-1.64868	-1.48920	-3.96007
H	0.46896	-1.70072	-2.67161
H	0.42987	-2.66702	-0.37808

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1544.1055477
Number of imaginary frequencies: 0

Compound 8'

Re	0.24648	-0.46037	-0.53124
N	0.30458	0.52639	-2.46986
C	-0.58720	0.62238	-3.45298

C	-0.10351	1.46737	-4.46343
C	1.13424	1.87952	-4.00193
N	1.35514	1.29981	-2.80520
N	2.50666	-0.71177	-0.81056
C	3.38243	-1.68943	-0.57308
C	4.66336	-1.31385	-1.00289
C	4.48554	-0.03954	-1.51835
N	3.18837	0.28990	-1.38841
N	0.81922	1.53964	0.09205
C	0.39152	2.30944	1.09246
C	1.12777	3.50221	1.12746
C	2.01500	3.38828	0.06814
N	1.80980	2.20079	-0.52965
B	2.47465	1.59886	-1.79088
N	0.46401	-0.85756	1.59841
C	-0.53079	-1.15104	2.49906
C	0.00532	-1.19851	3.75700
N	1.34605	-0.92826	3.61438
C	1.57558	-0.72817	2.29797
C	2.32691	-0.85611	4.67503
C	-1.57993	-0.16712	-0.34982
O	-2.72810	0.02535	-0.22481
H	-1.53150	0.08924	-3.37590
H	-0.59333	1.74379	-5.39233
H	1.87217	2.55133	-4.43318
H	3.05763	-2.61917	-0.11104
H	5.58202	-1.89088	-0.95309
H	5.18966	0.65491	-1.97001
H	-0.42688	1.96910	1.72342
H	1.01569	4.33613	1.81401
H	2.77146	4.07207	-0.30894
H	3.27680	2.38030	-2.25841
H	-1.55700	-1.29905	2.17314
H	-0.44508	-1.39398	4.72601
H	2.55126	-0.48001	1.88528
H	3.30675	-0.62243	4.24143
H	2.39543	-1.81695	5.20393
H	2.06236	-0.06670	5.39233
C	-4.61915	-3.94814	-0.74784
C	-3.47231	-3.85059	-0.02510
C	-2.25940	-3.33487	-0.61074
C	-2.29107	-2.92170	-2.00454
C	-3.53108	-3.05624	-2.72778
C	-4.64943	-3.54322	-2.12803
H	-5.52960	-4.33613	-0.28519
H	-3.44927	-4.16014	1.02363

C	-1.06805	-3.27943	0.08222
C	-1.13151	-2.47082	-2.60161
H	-3.55355	-2.74800	-3.77681
H	-5.58202	-3.63036	-2.69013
C	0.08001	-2.26633	-1.86690
C	0.11831	-2.70187	-0.47730
H	-1.13016	-2.28339	-3.67896
H	1.00817	-2.26521	-2.44758
H	-1.02050	-3.70668	1.08827
H	1.06120	-3.05870	-0.05064

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1544.0756089
Number of imaginary frequencies: 0

Compound 9

Cr	1.56318	0.61752	0.34702
C	2.98298	-0.09222	-0.49629
C	2.28708	0.58791	1.99863
C	2.17938	2.24506	-0.10307
C	0.10081	-0.45367	-0.75867
C	-0.35123	0.85772	-0.54119
C	-0.53699	1.20648	0.86504
C	-1.20957	0.16276	1.68008
C	-0.77658	-1.09509	1.47127
C	0.30281	-1.23258	0.46026
H	0.28465	-0.83691	-1.77131
H	-0.53643	1.54706	-1.37580
H	-0.78418	2.25348	1.08410
H	-2.07803	0.39057	2.32010
H	-1.26483	-1.97199	1.92773
H	0.75747	-2.22468	0.34073
O	2.75461	0.56500	3.08166
O	3.92151	-0.54564	-1.06482
O	2.59533	3.31244	-0.41502

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1615.8901156
Number of imaginary frequencies: 0

Compound 10

Mn	1.52787	0.06150	0.14358
C	2.66268	-1.16737	-0.47380
C	1.88452	-0.03865	1.88261
C	2.62784	1.38613	-0.31959
C	-0.06139	-0.59572	-1.00478
C	-0.08053	0.80868	-0.92000
C	-0.20217	1.31957	0.43290

C	-1.19353	0.62631	1.29760
C	-1.17530	-0.71168	1.21684
C	-0.16690	-1.26874	0.27666
H	0.07002	-1.11563	-1.95825
H	0.03515	1.44286	-1.80380
H	-0.09412	2.40164	0.56101
H	-1.92666	1.18813	1.88619
H	-1.89194	-1.35991	1.73237
H	-0.02930	-2.35502	0.27387
O	2.07542	-0.10495	3.02326
O	3.37741	-1.99226	-0.87397
O	3.31921	2.27231	-0.61642

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1722.5514265
Number of imaginary frequencies: 0

Compound 11

Fe	1.49448	0.06145	0.13723
C	2.63276	-1.18250	-0.47895
C	1.78383	-0.04104	1.90479
C	2.59756	1.40070	-0.32370
C	-0.05694	-0.59510	-1.02471
C	-0.07612	0.81092	-0.93959
C	-0.20206	1.32644	0.39709
C	-1.14306	0.62545	1.30494
C	-1.12483	-0.71070	1.22407
C	-0.16661	-1.27127	0.23987
H	0.11107	-1.11294	-1.97105
H	0.07622	1.44347	-1.81631
H	-0.07618	2.40407	0.53002
H	-1.81640	1.19086	1.95154
H	-1.78148	-1.36804	1.79667
H	-0.01127	-2.35324	0.24211
O	1.94765	-0.10665	3.03183
O	3.31423	-2.01888	-0.85435
O	3.25543	2.29419	-0.59523

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1835.215043
Number of imaginary frequencies: 0

Compound 12

C	-1.49931	-1.21825	0.34471
H	-1.36930	-2.24368	0.70084
C	-1.33739	-0.98455	-1.06084
H	-1.15140	-1.78537	-1.77925
C	-1.27684	0.38164	-1.42664

H	-1.04129	0.69891	-2.44442
C	-1.38780	1.29769	-0.32895
H	-1.16574	2.34933	-0.52895
C	-2.31105	0.98005	0.77595
H	-2.91620	1.75921	1.24482
C	-2.36853	-0.31687	1.12320
H	-3.02543	-0.70531	1.90471
C	1.80526	-1.21596	0.27339
C	2.14941	-0.32957	-0.77663
C	1.90291	0.98732	-0.31654
C	1.50221	0.92257	1.06397
C	1.44189	-0.43846	1.42839
H	2.02382	1.90096	-0.89646
H	2.46111	-0.61213	-1.78034
H	1.83747	-2.30347	0.22928
H	1.14766	-0.83486	2.39800
H	1.26322	1.77249	1.69988
Co	0.12331	-0.06160	-0.11119

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1807.9559646
Number of imaginary frequencies: 0

Compound 13

C	-1.59248	-1.29897	0.01604
H	-1.43163	-2.37787	0.09305
C	-1.46471	-0.71153	-1.29482
H	-1.29523	-1.29396	-2.20244
C	-1.46471	0.71147	-1.29485
H	-1.29523	1.29385	-2.20251
C	-1.59248	1.29898	0.01597
H	-1.43163	2.37788	0.09293
C	-2.53154	0.66999	0.97632
H	-3.19848	1.28080	1.58839
C	-2.53154	-0.66994	0.97635
H	-3.19848	-1.28072	1.58845
C	1.82083	-1.14292	0.69771
C	2.28378	-0.70406	-0.58906
C	2.28377	0.70409	-0.58905
C	1.82082	1.14294	0.69772
C	1.60564	0.00001	1.52478
H	2.56240	1.35105	-1.41866
H	2.56242	-1.35101	-1.41867
H	1.72756	-2.18094	1.01367
H	1.31795	0.00000	2.57344
H	1.72753	2.18096	1.01368
Rh	0.12345	-0.00000	-0.12152

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –535.906971
Number of imaginary frequencies: 0

Compound 14

Ir	0.14100	-0.00000	-0.09377
C	-1.57706	-1.27561	0.06326
H	-1.41119	-2.35376	0.14925
C	-1.45889	-0.71261	-1.27718
H	-1.31653	-1.30221	-2.18496
C	-1.45889	0.71255	-1.27722
H	-1.31653	1.30211	-2.18503
C	-1.57706	1.27561	0.06320
H	-1.41119	2.35378	0.14914
C	-2.59983	0.66820	0.96167
H	-3.32214	1.28848	1.49651
C	-2.59983	-0.66815	0.96171
H	-3.32214	-1.28840	1.49658
C	1.86796	-1.14917	0.69123
C	2.29081	-0.70854	-0.60368
C	2.29079	0.70857	-0.60368
C	1.86794	1.14918	0.69124
C	1.65266	0.00000	1.52113
H	2.55018	1.35231	-1.44172
H	2.55020	-1.35227	-1.44173
H	1.78419	-2.18636	1.01124
H	1.39939	-0.00000	2.57845
H	1.78416	2.18637	1.01126

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –529.73578
Number of imaginary frequencies: 0

Compound 15

Cr	-0.15945	0.23817	-0.10247
C	1.10974	1.49621	0.34549
C	0.93382	-0.34628	-1.46528
C	0.65778	-0.95827	1.03546
O	1.87927	2.30290	0.62795
O	1.59179	-0.71160	-2.33494
O	1.14083	-1.71295	1.75644
C	-2.02654	-0.84633	-0.57364
C	-1.78072	0.12412	-1.57023
C	-2.04072	-0.45138	0.78252
H	-2.14493	-1.89512	-0.84327
C	-1.59865	1.48266	-1.22863
H	-1.71115	-0.18242	-2.61489

C	-1.86022	0.90208	1.14423
H	-2.17242	-1.20397	1.56123
C	-1.61615	1.85784	0.13303
H	-1.38820	2.22151	-2.00094
H	-1.85064	1.19530	2.19333
H	-1.41859	2.89476	0.40849

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1616.0214893
Number of imaginary frequencies: 0

Compound 16

C	-2.29661	-2.06822	0.63628
C	-1.51364	0.42918	0.69372
C	-4.02942	-0.15478	0.71270
O	-2.10608	-2.98336	-0.03309
O	-0.82614	1.09904	0.06089
O	-4.94263	0.14611	0.07799
Cr	-2.59829	-0.62713	1.74796
C	0.73733	-2.45664	3.50710
C	-0.59473	-2.76549	3.47207
C	-1.58334	-1.73437	3.48276
C	-1.15612	-0.36965	3.51413
C	0.24394	-0.08655	3.53364
C	1.16182	-1.10068	3.53825
H	-3.31567	-3.05949	3.32325
H	1.48239	-3.25447	3.50546
H	-0.92605	-3.80566	3.44244
C	-2.99130	-2.02077	3.39606
C	-2.14847	0.67150	3.45804
H	0.56499	0.95710	3.55187
H	2.22868	-0.87055	3.56021
C	-3.51199	0.36438	3.48344
C	-3.93684	-0.99273	3.45223
H	-1.82199	1.71180	3.43311
H	-4.25127	1.16520	3.46014
H	-5.00032	-1.22759	3.40509

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1769.4986647
Number of imaginary frequencies: 0

Compound 17

C	-3.41314	-1.87613	0.88043
C	-1.11197	-0.67899	0.88158
C	-3.25714	0.71701	0.66064
O	-3.89446	-2.75847	0.31632

O	-0.13023	-0.77068	0.28655
O	-3.64690	1.51214	-0.07763
Cr	-2.65634	-0.52150	1.86231
C	-1.76384	-1.45472	3.75512
C	-3.14932	-1.77530	3.71326
C	-4.14733	-0.79027	3.48353
C	-3.72892	0.55262	3.43256
C	-2.35359	0.90499	3.50966
C	-1.36783	-0.09430	3.58889
C	-1.05695	-2.69705	3.93627
C	-2.00177	-3.67846	3.99983
H	-5.20018	-1.05436	3.39246
H	-4.47248	1.33575	3.28152
H	-2.06145	1.95015	3.41153
H	-0.31085	0.17268	3.57597
H	0.01875	-2.82861	4.01068
H	-4.12098	-3.65346	3.80195
N	-3.26053	-3.13075	3.87428
H	-1.87860	-4.75250	4.11820

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –1747.4575184
Number of imaginary frequencies: 0

5. Optimized Cartesian coordinates for σ-complexes, transition state structures, and products

Benzene + cyclopentadiene (reactants - exo)

C	-2.08692	-0.57576	0.77283
C	-1.80046	0.58228	-0.13369
C	-1.36671	1.66054	0.81190
H	-1.06918	2.66222	0.50096
H	-1.14557	1.74114	2.97778
H	-2.42653	-1.55243	0.42733
H	-1.97643	-0.83873	2.93271
H	-2.69139	0.87940	-0.71680
H	-1.01530	0.34235	-0.87360
C	-1.40584	1.18749	2.07429
C	-1.85558	-0.20898	2.04990
C	1.62489	0.24810	-2.12208
C	1.87259	0.87825	-0.90264
C	1.68924	0.18277	0.29301
C	1.26184	-1.14417	0.26905
C	1.01754	-1.77640	-0.95057
C	1.19691	-1.08063	-2.14608
H	1.76589	0.79350	-3.05806
H	2.20384	1.91900	-0.88296
H	1.86774	0.68058	1.24790
H	1.10629	-1.68352	1.20521
H	0.67911	-2.81487	-0.96845
H	1.00305	-1.57487	-3.10083

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –425.9068602
Gibbs free energy correction at ωB97X-D/def2-SVP(a.u.): 0.156211
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –426.3613515
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –425.5501098
Number of imaginary frequencies: 0

Benzene + cyclopentadiene (reactants - endo)

C	1.36554	0.89796	1.10686
C	2.45123	0.10948	0.43760
C	2.20815	-1.29053	0.91824
H	2.81547	-2.15033	0.63416
H	0.72277	-2.16733	2.24680
H	1.21780	1.96982	0.97628
H	-0.25501	0.35226	2.45287
H	3.45894	0.47218	0.71089
H	2.38586	0.18276	-0.66297

C	1.14127	-1.29513	1.74213
C	0.61494	0.06987	1.85915
C	-2.22318	1.12105	-0.42814
C	-1.26352	1.59513	-1.32131
C	-0.36177	0.70837	-1.91071
C	-0.41896	-0.65094	-1.60630
C	-1.37712	-1.12419	-0.71093
C	-2.27958	-0.23904	-0.12299
H	-2.92970	1.81452	0.03380
H	-1.21742	2.66020	-1.56000
H	0.38995	1.08055	-2.61103
H	0.29188	-1.34509	-2.06016
H	-1.41415	-2.18756	-0.46499
H	-3.02964	-0.61033	0.57922

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –425.9054269
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.154081
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –426.3598221
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –425.5488272
Number of imaginary frequencies: 0

Benzene + cyclopentadiene (Transition state - exo)

C	-2.07147	-1.63688	0.71075
C	-2.07881	-0.41670	-0.16713
C	-1.37026	0.54276	0.74770
H	-1.14781	1.57283	0.46092
H	-1.52392	0.74895	2.96070
H	-2.48901	-2.59385	0.39034
H	-2.33866	-1.78250	2.91783
H	-3.12474	-0.07817	-0.29004
H	-1.64058	-0.54077	-1.16525
C	-1.71317	0.15839	2.06303
C	-2.13907	-1.16522	2.04060
C	0.96488	-0.61383	-1.86005
C	0.99264	0.07824	-0.68621
C	0.45517	-0.48133	0.53131
C	0.01037	-1.86317	0.50799
C	0.13277	-2.59364	-0.73131
C	0.52536	-1.97970	-1.88310
H	1.33979	-0.15527	-2.77803
H	1.41066	1.08794	-0.65396
H	0.87542	-0.09685	1.46085
H	0.11815	-2.44884	1.42113
H	-0.11699	-3.65801	-0.73412
H	0.57152	-2.54248	-2.81834

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –425.8451167
Gibbs free energy correction(a.u.) at ωB97X-D/def2-SVP: 0.164652
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –426.2951466
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –425.4910287
Number of imaginary frequencies: 1

Benzene + cyclopentadiene (Transition state - endo)

C	0.90266	1.08139	0.81537
C	1.78108	-0.05945	0.37061
C	0.88513	-1.21247	0.74321
H	1.15706	-2.25415	0.55791
H	-0.43524	-1.43584	2.51965
H	1.19036	2.12840	0.69555
H	-0.41504	1.21286	2.60289
H	2.67383	-0.08678	1.02249
H	2.12124	-0.02923	-0.67276
C	0.16582	-0.78999	1.87925
C	0.17643	0.59941	1.92292
C	-2.74826	0.70653	-0.01806
C	-1.65638	1.39855	-0.43929
C	-0.43082	0.71678	-0.77912
C	-0.44151	-0.72875	-0.82449
C	-1.67727	-1.41232	-0.52782
C	-2.75897	-0.73206	-0.06343
H	-3.65346	1.23743	0.28630
H	-1.67760	2.49053	-0.48707
H	0.24065	1.24026	-1.46421
H	0.22245	-1.21802	-1.54146
H	-1.71465	-2.49869	-0.64424
H	-3.67212	-1.26756	0.20726

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –425.8425095
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.163643
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –426.2924147
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –425.4883001
Number of imaginary frequencies: 1

Benzene + cyclopentadiene (Product - exo)

C	-1.27627	-0.77623	0.56301
C	-1.54747	0.50143	-0.24821
C	-0.59084	1.35672	0.59878
H	-0.52052	2.42548	0.35635
H	-0.97720	1.66259	2.86724
H	-1.83918	-1.67801	0.28753
H	-1.79061	-0.86864	2.82479

H	-2.59233	0.83604	-0.17892
H	-1.24792	0.42289	-1.30446
C	-1.06867	1.01322	1.99502
C	-1.47825	-0.26134	1.97365
C	1.68487	0.26125	-1.92452
C	1.48020	1.03665	-0.85187
C	0.76017	0.57319	0.38364
C	0.28032	-0.92002	0.35859
C	0.60773	-1.67828	-0.89743
C	1.23618	-1.13499	-1.94795
H	2.20784	0.65774	-2.79826
H	1.83685	2.07158	-0.84862
H	1.41789	0.75837	1.24749
H	0.69867	-1.47977	1.20993
H	0.29484	-2.72680	-0.92913
H	1.43888	-1.73508	-2.83842

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –425.8942482
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.168771
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –426.3417532
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –425.5365039
Number of imaginary frequencies: 0

Benzene + cyclopentadiene (Product - endo)

C	1.27084	1.10293	0.31834
C	2.28721	-0.01860	0.04894
C	1.25412	-1.13955	0.24794
H	1.61195	-2.17528	0.17709
H	0.18994	-1.39987	2.29662
H	1.64409	2.13562	0.31243
H	0.20970	1.25006	2.37982
H	3.09466	-0.04802	0.79417
H	2.71650	0.01004	-0.96521
C	0.65216	-0.72386	1.57669
C	0.66213	0.61372	1.61868
C	-2.23899	0.76332	-0.39335
C	-1.11061	1.45937	-0.58222
C	0.22119	0.80766	-0.81614
C	0.20952	-0.75810	-0.86529
C	-1.13197	-1.40328	-0.67209
C	-2.24993	-0.70371	-0.43940
H	-3.18268	1.28494	-0.21507
H	-1.12970	2.55368	-0.55857
H	0.63723	1.20528	-1.75736
H	0.62002	-1.10206	-1.82980

H	-1.16737	-2.49651	-0.71712
H	-3.20137	-1.22136	-0.29375

Electronic energy (a.u.) at ωB97X-D/def2-SVP:–425.8943196
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.168798
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –426.3411221
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –425.5361987
Number of imaginary frequencies: 0

p-nitro-aniline + cyclopentadiene (reactants - exo)

C	-0.91218	1.54839	1.66976
C	0.02082	1.57734	2.64356
C	1.22529	2.24326	2.13566
C	1.01935	2.61523	0.85526
H	-0.37075	1.55438	-0.43529
H	-0.08758	1.16839	3.64916
H	2.13668	2.40440	2.71400
C	-0.36725	2.22033	0.44607
H	-0.97362	3.10019	0.16196
C	1.86324	-0.20553	-1.18697
C	0.90860	-0.32907	-2.21853
C	-0.34234	-0.86733	-1.96375
C	-0.65754	-1.28631	-0.67277
C	0.27330	-1.19108	0.36135
C	1.52473	-0.66196	0.10374
H	1.15502	0.01514	-3.22552
H	-1.09039	-0.96041	-2.75069
H	2.24751	-0.56549	0.91582
N	-1.99183	-1.80491	-0.39161
O	-2.26566	-2.06485	0.76305
O	-2.75583	-1.94024	-1.32568
N	3.07460	0.38164	-1.42249
H	3.79658	0.32087	-0.72010
H	3.38309	0.52001	-2.37330
H	-1.90571	1.10407	1.73454
H	1.72793	3.12442	0.20172
H	-0.00514	-1.52115	1.36095

Electronic energy (a.u.) at ωB97xd/def2-SVP (a.u.) : –685.4982238
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.171609
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –686.2571581
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –685.0657224
Number of imaginary frequencies: 0

p-nitro-aniline + cyclopentadiene (reactants - endo)

C	0.65672	2.19520	2.23219
C	1.10793	2.61041	1.03093
C	0.05758	2.41254	0.02628
C	-1.02801	1.87970	0.62337
H	-0.84872	0.63601	2.39468
H	2.09468	3.02724	0.82267
H	0.15773	2.65320	-1.03298
C	-0.74744	1.69262	2.08402
H	-1.45703	2.25813	2.71528
C	1.78648	-0.28088	-1.60085
C	0.52283	-0.58350	-2.15109
C	-0.49689	-1.06831	-1.35284
C	-0.26951	-1.25750	0.00955
C	0.97473	-0.98721	0.57488
C	1.99470	-0.50638	-0.22532
H	0.34631	-0.42107	-3.21681
H	-1.47999	-1.29367	-1.76487
H	2.96497	-0.27433	0.21871
N	-1.36067	-1.71429	0.85880
O	-1.15569	-1.79024	2.05665
O	-2.41926	-1.98493	0.33056
N	2.77801	0.25019	-2.37971
H	3.72207	0.27071	-2.02277
H	2.68705	0.20931	-3.38427
H	1.20316	2.21465	3.17551
H	-1.96872	1.60868	0.14317
H	1.12339	-1.14193	1.64288

Electronic energy (a.u.) at ωB97xd/def2-SVP: –685.4990062
Gibbs free energy (a.u.) correction at ωB97X-D/def2-SVP: 0.172197
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –686.2570728
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –685.0662158
Number of imaginary frequencies: 0

p-nitro-aniline + cyclopentadiene (Transition state - exo)

C	0.68358	3.40874	0.78520
C	1.43526	3.65589	1.95631
C	2.64391	4.24691	1.59804
C	2.66876	4.39794	0.19989
H	1.09397	4.02580	-1.30905
H	1.17266	3.29851	2.95285
H	3.48714	4.42391	2.26730
C	1.24599	4.32917	-0.26586
H	0.78723	5.32685	-0.13261

C	3.30189	2.38438	-1.70704
C	2.38335	2.07437	-2.70052
C	1.13192	1.52183	-2.35829
C	0.79222	1.32256	-1.04615
C	1.63490	1.75802	0.04524
C	2.92983	2.27999	-0.31814
H	2.65054	2.19930	-3.75168
H	0.42704	1.21708	-3.13217
H	3.75260	2.13818	0.38365
N	-0.46599	0.68625	-0.72748
O	-0.76549	0.59463	0.45307
O	-1.16284	0.27555	-1.63662
N	4.55421	2.85009	-2.00703
H	5.24996	2.85828	-1.27446
H	4.90889	2.71088	-2.94277
H	-0.36275	3.09988	0.81324
H	3.45661	4.91176	-0.35479
H	1.55151	1.16938	0.95698

Electronic energy (a.u.) at ωB97xd/def2-SVP: –685.4452332
Gibbs free energy correction(a.u.) at ωB97X-D/def2-SVP: 0.179279
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –686.199347
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –685.0140307
Number of imaginary frequencies: 1

p-nitro-aniline + cyclopentadiene (Transition state - endo)

C	2.75524	4.40308	0.32725
C	1.83044	4.80752	-0.64495
C	0.59836	4.22909	-0.35183
C	0.72957	3.42809	0.80599
H	2.45770	3.23663	2.19085
H	2.07343	5.35279	-1.55711
H	-0.28226	4.26070	-0.99407
C	1.95979	3.94319	1.51445
H	1.66763	4.83169	2.10427
C	3.35082	2.31516	-1.62196
C	2.44094	1.96728	-2.60760
C	1.19445	1.39907	-2.25931
C	0.84540	1.23814	-0.94805
C	1.65798	1.77351	0.12262
C	2.96399	2.25567	-0.23690
H	2.71228	2.06480	-3.66074
H	0.50685	1.05149	-3.03099
H	3.77290	2.15523	0.49065
N	-0.41182	0.62008	-0.60985

O	-0.72266	0.58816	0.57204
O	-1.10188	0.16289	-1.50265
N	4.59740	2.79118	-1.92842
H	5.28580	2.84221	-1.19102
H	4.96411	2.62107	-2.85431
H	3.77996	4.77475	0.39003
H	-0.12842	3.01380	1.33910
H	1.55263	1.26382	1.08150

Electronic energy (a.u.) at ωB97xd/def2-SVP: –685.4439155
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP : 0.178712
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –686.1982654
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –685.0124854
Number of imaginary frequencies: 1

p-nitro-aniline + cyclopentadiene (Product - exo)

C	-0.75113	0.93692	1.21391
C	-0.03517	1.26925	2.50556
C	1.16823	1.75775	2.18194
C	1.25997	1.75795	0.66944
H	-0.42323	1.86629	-0.77506
H	-0.40907	1.03607	3.50333
H	1.98605	2.00916	2.85916
C	-0.20266	2.03438	0.29055
H	-0.53119	3.04137	0.58313
C	1.77603	0.12610	-1.22235
C	0.94590	-0.40846	-2.16442
C	-0.32024	-0.96472	-1.78781
C	-0.75894	-0.95667	-0.51172
C	-0.02015	-0.33294	0.63096
C	1.38221	0.24452	0.23152
H	1.26333	-0.46818	-3.20715
H	-0.94773	-1.44401	-2.54069
H	2.18004	-0.24169	0.81585
N	-2.00451	-1.62314	-0.19607
O	-2.32044	-1.67856	0.98231
O	-2.66947	-2.09785	-1.09787
N	3.00697	0.61791	-1.51959
H	3.64481	0.87421	-0.78091
H	3.39364	0.49789	-2.44459
H	-1.83678	0.81086	1.28010
H	2.02579	2.40849	0.22780
H	0.07832	-1.08264	1.42734

Electronic energy (a.u.) at ωB97xd/def2-SVP: –685.4955309
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.183783

Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –686.2465297
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –685.0588441
Number of imaginary frequencies: 0

p-nitro-aniline + cyclopentadiene (Product - endo)

C	1.35069	1.70060	0.86976
C	0.33936	2.36546	-0.04443
C	-0.86594	1.88471	0.28378
C	-0.67099	0.90083	1.42014
H	0.97945	0.89058	2.90402
H	0.58665	3.01448	-0.88492
H	-1.80898	2.06774	-0.23206
C	0.51696	1.54620	2.14943
H	0.26240	2.51359	2.60400
C	1.86176	0.05116	-1.02461
C	1.04508	-0.50932	-1.96207
C	-0.23295	-1.04437	-1.59248
C	-0.69765	-1.00359	-0.32625
C	0.03542	-0.36492	0.81045
C	1.44381	0.19411	0.41713
H	1.37296	-0.58932	-3.00024
H	-0.85449	-1.52964	-2.34664
H	2.21921	-0.30088	1.02687
N	-1.96058	-1.63673	-0.02099
O	-2.29760	-1.66223	1.15305
O	-2.62134	-2.11481	-0.92440
N	3.08982	0.55397	-1.31462
H	3.71409	0.83310	-0.57295
H	3.48859	0.42772	-2.23364
H	2.32521	2.19841	0.96243
H	-1.55708	0.64363	2.00915
H	0.14000	-1.10424	1.61844

Electronic energy (a.u.) at ωB97xd/def2-SVP: –685.49683
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.183756
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –686.2473162
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –685.0600698
Number of imaginary frequencies: 0

1 + NMN (reactants - exo)

W	0.76533400	-0.15043400	-0.30291900
P	0.88541800	-2.63526800	0.05764900
O	-0.03415900	-0.66515200	-3.10106800
N	1.56634700	0.18171600	1.85616100
N	2.70241300	0.87252500	2.04900400
N	2.95211100	-0.27454000	-0.80651300

N	3.89224400	0.41211000	-0.13539800
N	1.42442000	2.00121500	-0.51661800
N	2.52918700	2.46280900	0.09922100
N	0.27670900	-0.43313400	-1.97292300
C	-1.27176000	-0.57437700	0.59631800
C	-1.10922800	0.85781000	0.33493700
C	-1.97157900	1.46591300	-0.66696400
C	-2.78201800	0.72178900	-1.46575300
C	-2.93237800	-0.68800400	-1.22288600
C	-2.27748200	-1.27955900	-0.18951200
C	2.98546700	0.94472100	3.36042300
C	1.99368100	0.27358000	4.05920700
C	1.12530200	-0.18386600	3.06132100
C	5.09573800	0.21298000	-0.70219700
C	4.93538600	-0.63936500	-1.78387700
C	3.56011000	-0.90387100	-1.81167100
C	2.73906700	3.74853000	-0.24210800
C	1.73558300	4.13904300	-1.11255300
C	0.93734500	2.99515000	-1.25538500
C	0.17377200	-3.57129000	-1.34058000
C	0.07877500	-3.39900000	1.52063600
C	2.57343200	-3.34327900	0.23145000
B	3.46695000	1.50870300	0.87021400
H	-1.18719100	-0.91325700	1.63564900
H	4.43931600	2.10402000	1.28236700
H	-0.84021300	1.50190100	1.18170300
H	-1.97306500	2.55498700	-0.76211200
H	-3.39174800	1.20531500	-2.23160100
H	-3.65265200	-1.26157200	-1.81043900
H	-2.52519800	-2.31271900	0.07348400
H	3.87094100	1.47250700	3.70581200
H	1.90851700	0.13961500	5.13332700
H	0.20154000	-0.74890600	3.16054900
H	5.98045100	0.70512900	-0.30576800
H	5.69972100	-1.00394700	-2.46345400
H	2.97573000	-1.49855100	-2.51146700
H	3.59300700	4.29180100	0.15499900
H	1.60091400	5.10902200	-1.58158100
H	0.04623100	2.83398700	-1.85704300
H	-0.87984600	-3.28145700	-1.45627600
H	0.68855900	-3.27811700	-2.26625600
H	0.25438200	-4.65794000	-1.19149300
H	0.51991200	-2.98482900	2.43852400
H	-0.99868900	-3.19114600	1.52144600
H	0.23108100	-4.48838000	1.51690600
H	3.09860900	-2.81751000	1.04275600

H	3.14854800	-3.19509900	-0.69092900
H	2.53099900	-4.41853200	0.45961000
C	-5.30572000	-0.63907200	0.87855100
C	-4.35258600	0.06658100	1.79718300
H	-3.81216800	-0.45915800	2.58142500
C	-4.31312100	1.35812600	1.46510800
H	-3.73149900	2.16550300	1.90508200
C	-5.24225000	1.58321500	0.30751000
N	-5.79266700	0.33880000	0.01514900
O	-5.50071600	2.61104500	-0.26298800
C	-6.68982800	0.08867700	-1.08254800
H	-7.51617300	0.81242500	-1.07256500
H	-6.16470600	0.16814800	-2.04694500
H	-7.08397800	-0.92905200	-0.96916400
O	-5.62158400	-1.80134600	0.87497900

Electronic energy (a.u.) at ωB97xd/def2-SVP: –1989.952497
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.458152
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: −1989.95249741
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –1988.332061
Number of imaginary frequencies: 0

1 + NMN (reactants - endo)

W	-0.68132000	0.40294700	-0.37541300
P	-1.19305200	2.35877900	1.11615400
O	-1.23496200	2.10356200	-2.72930600
N	-0.40255400	-0.92425400	1.52199500
N	-1.18566900	-2.00439100	1.69450600
N	-2.84624100	-0.14379000	-0.13532900
N	-3.24441400	-1.31533300	0.38789600
N	-0.85826400	-1.63247300	-1.34313300
N	-1.48110400	-2.65143900	-0.72167800
N	-0.99668700	1.40046800	-1.79436200
C	1.37969500	1.22390000	0.03767100
C	1.45937900	0.01301600	-0.78538300
C	2.00826100	0.13338000	-2.12656200
C	2.30194300	1.34148000	-2.67506900
C	2.20050400	2.53917800	-1.88118300
C	1.82814000	2.46794600	-0.57747900
C	-0.86019900	-2.63606100	2.83516900
C	0.17921500	-1.94351100	3.43588500
C	0.43059400	-0.87633100	2.56475400
C	-4.58547100	-1.40572800	0.33817800
C	-5.08218600	-0.24611200	-0.23723200
C	-3.93902700	0.50898600	-0.52955100

C	-1.49788400	-3.73348600	-1.52290700
C	-0.86410400	-3.40800300	-2.71034600
C	-0.48505800	-2.06847400	-2.54376400
C	-1.33154800	3.92692900	0.18828800
C	-0.05421800	2.78044100	2.49375300
C	-2.77970200	2.27350300	2.04149000
B	-2.20750100	-2.43887600	0.62526200
H	1.61390100	1.13994200	1.10220000
H	-2.76372000	-3.45777200	0.97570200
H	1.66574300	-0.93760700	-0.28115700
H	2.21121700	-0.78387500	-2.68550900
H	2.67968200	1.40622000	-3.69779800
H	2.49737000	3.49639100	-2.31573600
H	1.87613600	3.36900900	0.04318800
H	-1.38830100	-3.53746600	3.13620200
H	0.68892200	-2.17600000	4.36601100
H	1.19977700	-0.10962000	2.64130000
H	-5.09205200	-2.29662800	0.70114200
H	-6.11948700	0.00934300	-0.43142400
H	-3.84486500	1.47772300	-1.01689400
H	-1.96547700	-4.65736900	-1.19150600
H	-0.70062400	-4.04485200	-3.57439800
H	0.02872900	-1.39609900	-3.22634100
H	-0.38323300	4.11141500	-0.33502500
H	-2.10578100	3.81631000	-0.58389400
H	-1.57375300	4.77457700	0.84600500
H	0.01855800	1.92460100	3.17977100
H	0.95157000	3.00598500	2.11766700
H	-0.43232700	3.65057500	3.05036100
H	-2.80860500	1.33361400	2.61258800
H	-3.62948600	2.27092700	1.34766700
H	-2.88204500	3.12388400	2.73172700
C	4.55406900	-1.14454600	-0.44868800
C	4.92769600	0.28437800	-0.71553100
H	5.34382500	0.60568000	-1.66753200
C	4.64348200	1.00586700	0.36984900
H	4.76323800	2.07389600	0.53659500
C	4.04887800	0.09776200	1.40503300
N	4.06283400	-1.17626600	0.85730200
O	3.62033700	0.38763000	2.49691300
C	3.49876100	-2.34763700	1.47884400
H	3.49238000	-2.19578200	2.56535100
H	2.46426900	-2.52334700	1.14185300
H	4.10766600	-3.22441400	1.22370600
O	4.64151200	-2.09663500	-1.17780400

Electronic energy (a.u.) at ωB97xd/def2-SVP: –1989.959408
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.460797
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: −1989.95940825
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –1988.337154
Number of imaginary frequencies: 0

1 + NMN (Transition state - exo)

W	-0.69876400	0.13741100	-0.26401200
P	-0.80937000	2.63556000	0.03166800
O	0.15021400	0.63434700	-3.04887100
N	-1.65897800	-0.13647400	1.83847900
N	-2.82203700	-0.79934200	1.96115000
N	-2.84546300	0.27138900	-0.92748100
N	-3.84504900	-0.38485100	-0.31498500
N	-1.36630300	-2.01209900	-0.45469700
N	-2.52587100	-2.44195400	0.07672300
N	-0.15032000	0.39928600	-1.91761100
C	1.24072600	0.56993800	0.77423400
C	1.10419400	-0.86379600	0.49731200
C	2.14617800	-1.42598800	-0.36710000
C	2.74198100	-0.62803600	-1.36078000
C	2.86951600	0.72478500	-1.10502200
C	2.40582200	1.19880400	0.13629200
C	-3.20306900	-0.83450800	3.24889400
C	-2.25170500	-0.16732600	4.00509700
C	-1.30147200	0.24815100	3.06573400
C	-4.99460500	-0.19542100	-0.98670100
C	-4.73560600	0.61959500	-2.07828800
C	-3.36003400	0.87124000	-2.00059000
C	-2.70141200	-3.74642100	-0.20453300
C	-1.61715100	-4.18354200	-0.94740200
C	-0.80764800	-3.04711500	-1.07804400
C	0.10680300	3.52428700	-1.27507500
C	-0.17684000	3.39866400	1.57604700
C	-2.48278900	3.39213400	-0.03769600
B	-3.50922700	-1.45723100	0.74689200
H	1.10114800	0.88510100	1.81522800
H	-4.51544300	-2.03186500	1.10242800
H	0.81344500	-1.50909700	1.33635700
H	2.20189100	-2.51303400	-0.46901100
H	3.25836500	-1.09093100	-2.20359200
H	3.49309300	1.35822100	-1.73872700
H	2.66953600	2.22049400	0.42726800
H	-4.12269200	-1.33664800	3.53878900
H	-2.24306100	-0.01032200	5.07940100
H	-0.37603200	0.79653200	3.22361600

H	-5.91446900	-0.66761000	-0.65046700
H	-5.43693900	0.96760400	-2.83057200
H	-2.71134200	1.43179700	-2.67161500
H	-3.58910100	-4.27029800	0.14127100
H	-1.43733000	-5.17928400	-1.34113300
H	0.14202400	-2.92101800	-1.59204900
H	1.17228200	3.26894700	-1.19730000
H	-0.23645700	3.17102700	-2.25774100
H	-0.02331700	4.61331000	-1.19499900
H	-0.75117600	3.02150300	2.43414900
H	0.88218500	3.14986200	1.72121900
H	-0.28305600	4.49254700	1.53285900
H	-3.13544100	2.89117900	0.69244800
H	-2.92367000	3.25394400	-1.03270600
H	-2.43848000	4.46783500	0.18785100
C	5.12244000	0.65555000	0.73594200
C	3.88592400	0.16360400	1.40254500
H	3.51636800	0.67246300	2.29057900
C	3.76960900	-1.20210800	1.14034600
H	3.28595100	-1.93505100	1.78232900
C	4.92739700	-1.60474200	0.29719300
N	5.63138800	-0.43010900	0.02266500
O	5.23941600	-2.69890200	-0.10856200
C	6.77980500	-0.36640000	-0.84235500
H	7.43013900	-1.23278700	-0.66101800
H	6.48166500	-0.37018100	-1.90256400
H	7.31834700	0.56465300	-0.62434100
O	5.61496900	1.75910300	0.76036400

Electronic energy (a.u.) at ωB97xd/def2-SVP: –1989.925831
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.464007
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: −1989.92583080
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –1988.306531
Number of imaginary frequencies: 1

1 + NMN (Transition state - endo)

W	-0.59576100	0.34357500	-0.37793000
P	-0.66975900	2.48947400	0.94064100
O	-0.89737200	1.97522300	-2.82293200
N	-0.62679800	-0.84370200	1.62595000
N	-1.60314800	-1.73905600	1.85563900
N	-2.83011200	0.27600800	-0.13512800
N	-3.46766400	-0.74461400	0.46313300
N	-1.18468200	-1.68067200	-1.18554400
N	-2.01433200	-2.49661700	-0.50966800
N	-0.73917800	1.28788900	-1.85846000

C	1.55727100	0.73110000	0.04697500
C	1.40024000	-0.50564400	-0.73202500
C	2.08171800	-0.50771100	-2.02357300
C	2.24191500	0.69755200	-2.73745900
C	2.39120800	1.85898000	-2.00780500
C	2.38980900	1.74891100	-0.60120600
C	-1.42751600	-2.32058500	3.05373700
C	-0.28959300	-1.78489600	3.63713600
C	0.17473400	-0.86146100	2.69379000
C	-4.79752600	-0.56203400	0.38151400
C	-5.03710500	0.62550700	-0.29323800
C	-3.75966600	1.10462000	-0.60949000
C	-2.21876500	-3.62536100	-1.21346900
C	-1.49673500	-3.54231700	-2.39261800
C	-0.86507000	-2.29349300	-2.32301500
C	-0.31421900	3.94850300	-0.10043700
C	0.44422900	2.70627100	2.38333600
C	-2.28017300	2.92275800	1.71364300
B	-2.68889800	-2.03760200	0.80145800
H	1.77192900	0.62406200	1.11331200
H	-3.44399200	-2.89044100	1.21584900
H	1.44849300	-1.45993200	-0.19297500
H	2.15126900	-1.45992200	-2.55598200
H	2.42953000	0.68307700	-3.81304600
H	2.70435500	2.78702700	-2.49098300
H	2.67987900	2.61773100	-0.00272800
H	-2.12259400	-3.07836300	3.40663200
H	0.14444100	-2.02859600	4.60207900
H	1.05297500	-0.22147000	2.74058600
H	-5.48184900	-1.29882000	0.79502300
H	-5.99691700	1.07165900	-0.53534700
H	-3.46175900	1.98805100	-1.17144200
H	-2.86664000	-4.40736100	-0.82529800
H	-1.43424100	-4.27818700	-3.18845700
H	-0.20207100	-1.80477600	-3.03257300
H	0.71779600	3.88223300	-0.46896800
H	-0.97217500	3.92657300	-0.98088100
H	-0.45216100	4.88718700	0.45569700
H	0.16424600	1.98582200	3.16531100
H	1.49452700	2.53350800	2.11304700
H	0.34145400	3.72278500	2.79077900
H	-2.63202800	2.07438600	2.31876700
H	-3.03322600	3.12144000	0.94089300
H	-2.18180400	3.81279800	2.35260200
C	4.07588700	-1.62748900	-0.32302400
C	4.20657800	-0.47183700	-1.24657600

H	4.64947200	-0.62121700	-2.22820700
C	4.31020700	0.68774000	-0.47054600
H	4.88704600	1.57203700	-0.73215900
C	4.21782900	0.28228700	0.96204000
N	4.03700300	-1.09680600	0.97035200
O	4.23494700	0.97904800	1.95254100
C	3.75641800	-1.87989900	2.14390000
H	3.91565600	-1.23897100	3.02065200
H	2.71683900	-2.24545400	2.13909500
H	4.42702000	-2.74885300	2.19162300
O	3.98667700	-2.80585300	-0.57041500

Electronic energy (a.u.) at ωB97xd/def2-SVP: –1989.928305
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.465971
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: −1989.92830522
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –1988.307725
Number of imaginary frequencies: 01

1 + NMN (Product - exo)

W	0.67289700	-0.12552400	-0.24484800
P	0.74588900	-2.62317800	0.04959500
O	-0.04768300	-0.66693400	-3.05644000
N	1.68833400	0.12963600	1.83840300
N	2.86716100	0.76843300	1.93932000
N	2.81966800	-0.28461500	-0.94512200
N	3.84273800	0.35568300	-0.35605900
N	1.37173000	2.01597600	-0.42084100
N	2.55351200	2.42560400	0.07537500
N	0.16379100	-0.40154300	-1.90775400
C	-1.22907200	-0.53944700	0.83052700
C	-1.09615900	0.87779900	0.53467000
C	-2.32117700	1.41312400	-0.22911300
C	-2.59794300	0.55581000	-1.43536400
C	-2.72229300	-0.74654400	-1.16745400
C	-2.55948600	-1.09721100	0.28810000
C	3.27537900	0.79043900	3.21894900
C	2.32683600	0.13917100	3.99225600
C	1.34859100	-0.25224600	3.07135800
C	4.97149400	0.15813600	-1.05989900
C	4.67324500	-0.64685600	-2.14898000
C	3.29704300	-0.88277600	-2.03587500
C	2.72104300	3.73831100	-0.16804700
C	1.60758600	4.20260200	-0.84930300
C	0.78904200	3.07315200	-0.98183200
C	-0.27360000	-3.49556200	-1.19158600
C	0.19508400	-3.36571400	1.63335100

C	2.38889500	-3.42757400	-0.13479300
B	3.54107300	1.42485100	0.71618600
H	-1.08326300	-0.84163000	1.87643700
H	4.55986400	1.98675100	1.05665600
H	-0.80472700	1.53756700	1.36499300
H	-2.23981600	2.47992200	-0.47528200
H	-2.64902500	0.97107400	-2.44311600
H	-2.88900000	-1.50557600	-1.93363700
H	-2.68952800	-2.17168700	0.48094300
H	4.21050600	1.27336900	3.49139900
H	2.33738100	-0.02213200	5.06592200
H	0.41504900	-0.78149500	3.24484700
H	5.90551300	0.61777100	-0.74589700
H	5.34978800	-0.99801000	-2.92224800
H	2.62116800	-1.42467200	-2.69581200
H	3.62323700	4.24888000	0.15962500
H	1.41439400	5.21156900	-1.20077200
H	-0.18549200	2.96733300	-1.45142100
H	-1.33364000	-3.30088600	-0.98288900
H	-0.05290600	-3.08500800	-2.18755000
H	-0.08990100	-4.57972000	-1.17540100
H	0.83845000	-3.01105000	2.45105200
H	-0.84216400	-3.07594000	1.84561300
H	0.25815700	-4.46263800	1.58275200
H	3.10908000	-2.94236000	0.54020400
H	2.75671500	-3.30744600	-1.16152900
H	2.33081700	-4.50065800	0.10041300
C	-5.05797200	-0.66798000	0.63008700
C	-3.65205900	-0.30149600	1.06722600
H	-3.56050300	-0.52270600	2.14145300
C	-3.51221400	1.19854300	0.75647000
H	-3.34258100	1.80461900	1.65890300
C	-4.84867000	1.59927500	0.16042400
N	-5.66927700	0.47852000	0.13989200
O	-5.17914200	2.68479400	-0.24549600
C	-7.00201300	0.49901300	-0.41289200
H	-7.58997600	1.30330400	0.04956700
H	-6.96667300	0.67367400	-1.49807800
H	-7.46403000	-0.47506600	-0.21155500
O	-5.57668600	-1.75544400	0.67895000

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1989.998050
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.471110
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: −1989.99804967
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1988.36969
Number of imaginary frequencies: 0

1 + NMN (Product - endo)

W	-0.59661800	0.30806800	-0.35422400
P	-0.65119500	2.47917000	0.91798700
O	-1.01527200	1.92071400	-2.79340800
N	-0.69294400	-0.84667100	1.67172400
N	-1.70842300	-1.69448600	1.91290900
N	-2.84819400	0.28685800	-0.14730600
N	-3.52642900	-0.70060700	0.45961700
N	-1.20964700	-1.73189900	-1.10391200
N	-2.08426100	-2.50514600	-0.43509500
N	-0.77356100	1.23553200	-1.84050300
C	1.53652800	0.68230100	0.09630100
C	1.38128100	-0.55282300	-0.65527300
C	2.27071500	-0.56561400	-1.91084700
C	2.03157700	0.68109700	-2.72218100
C	2.17539900	1.81819400	-2.03748700
C	2.54247500	1.62656600	-0.58880200
C	-1.56692700	-2.25542300	3.12536900
C	-0.41176000	-1.75574800	3.70650000
C	0.09997300	-0.87660600	2.74540200
C	-4.84880800	-0.49047400	0.33418100
C	-5.04013300	0.68318600	-0.37930600
C	-3.74278900	1.12334600	-0.67175000
C	-2.26671200	-3.66392100	-1.09414000
C	-1.48300500	-3.64562300	-2.23649200
C	-0.83735000	-2.40304400	-2.19128600
C	-0.21852000	3.90808500	-0.13726400
C	0.42921100	2.69380800	2.38465800
C	-2.27129900	2.98028900	1.62879400
B	-2.78215300	-1.99724200	0.84663400
H	1.75737100	0.59225300	1.16585700
H	-3.56102900	-2.82558600	1.26721700
H	1.43545400	-1.49773600	-0.09555100
H	2.15950500	-1.49045300	-2.49219500
H	1.71162300	0.64247000	-3.76484900
H	1.98552900	2.80500800	-2.46338600
H	2.66747400	2.57417400	-0.04617300
H	-2.29545800	-2.97619500	3.48818500
H	0.00368100	-1.99626200	4.68038900
H	1.00584600	-0.27600800	2.78066700
H	-5.56202500	-1.19971700	0.74711300
H	-5.98165800	1.14450600	-0.66157700
H	-3.40632000	1.97941900	-1.25461800
H	-2.94301800	-4.41991700	-0.70293100
H	-1.38915800	-4.41938400	-2.99229700

H	-0.12589000	-1.95882700	-2.88254000
H	0.84730400	3.85272300	-0.39329400
H	-0.78746500	3.84345200	-1.07608900
H	-0.42444200	4.86182100	0.37017400
H	0.13851900	1.97019400	3.15970200
H	1.48301400	2.52516100	2.12528600
H	0.31753600	3.70963900	2.79142700
H	-2.66720000	2.16050200	2.24593600
H	-2.99319600	3.17644200	0.82604200
H	-2.16778000	3.88598700	2.24461800
C	4.08786100	-1.56249700	-0.41379200
C	3.74072300	-0.45417200	-1.38915100
H	4.43835400	-0.51119900	-2.23719800
C	3.89338500	0.84683600	-0.58018200
H	4.69971900	1.49016300	-0.96223100
C	4.26466400	0.39856200	0.82175200
N	4.37449100	-0.98381400	0.81883000
O	4.41464200	1.09424800	1.79762600
C	4.65567800	-1.76550100	1.99821400
H	5.02059300	-1.08527100	2.77732400
H	3.74559300	-2.27421100	2.35129300
H	5.41152300	-2.52804000	1.76893400
O	4.10740900	-2.74955700	-0.61782000

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1990.000837
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.470851
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: −1990.00083665
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1988.37176
Number of imaginary frequencies: 0

2 + NMN (reactants - exo)

Re	0.05467	0.75126	0.14064
C	-0.23039	-1.43496	0.27720
C	-0.30543	-1.03288	-1.11920
C	-1.57433	-1.21229	-1.80225
C	-2.70186	-1.59288	-1.13880
C	-2.63253	-1.96515	0.24474
C	-1.43725	-1.95373	0.89758
N	0.12567	1.69394	-1.82217
C	-0.78129	1.81544	-2.78835
C	-0.26722	2.59022	-3.83850
C	1.00648	2.93302	-3.41948
N	1.21749	2.38119	-2.20829
N	2.28076	0.33726	-0.20411
C	3.09056	-0.69614	0.03029
C	4.38227	-0.42240	-0.44198

C	4.28159	0.85128	-0.97933
N	3.01562	1.27628	-0.82089
N	0.78453	2.74102	0.68728
C	0.43872	3.56940	1.67187
C	1.26176	4.70424	1.65453
C	2.11240	4.49345	0.57977
N	1.80618	3.30747	0.02451
B	2.38742	2.62458	-1.23682
N	0.33293	0.42398	2.27739
C	-0.63897	0.22019	3.22595
C	-0.05370	0.17490	4.46143
N	1.29393	0.35622	4.25563
C	1.47934	0.50310	2.92603
C	2.32172	0.39474	5.27319
C	-1.73946	1.17190	0.37554
O	-2.86672	1.44414	0.53483
H	0.69981	-1.87270	0.65770
H	0.58778	-1.14395	-1.74523
H	-1.61215	-1.05684	-2.88368
H	-3.64678	-1.69172	-1.67751
H	-3.52772	-2.33418	0.75043
H	-1.37102	-2.35914	1.91101
H	-1.75573	1.34743	-2.67351
H	-0.75973	2.86562	-4.76622
H	1.77730	3.53728	-3.89122
H	2.71269	-1.58973	0.52228
H	5.25859	-1.06274	-0.40437
H	5.02050	1.48399	-1.46484
H	-0.38651	3.30933	2.33159
H	1.22816	5.56395	2.31715
H	2.90716	5.10831	0.16462
H	3.22914	3.33193	-1.74981
H	-1.68495	0.12465	2.94706
H	-0.47338	0.03301	5.45324
H	2.45009	0.67586	2.46604
H	3.29530	0.55093	4.79322
H	2.34996	-0.55294	5.82865
H	2.13856	1.22018	5.97506
C	-2.26504	-4.46455	-2.36116
C	-0.83806	-4.29193	-1.92984
C	-0.73563	-4.63802	-0.64541
C	-2.08888	-5.05687	-0.15039
H	-0.06941	-3.93142	-2.61016
H	0.13997	-4.63565	0.00006
N	-2.94848	-4.91976	-1.23545
C	-4.36828	-5.14956	-1.18007

H	-4.57712	-6.08702	-0.64744
H	-4.88311	-4.32664	-0.65989
H	-4.74253	-5.21149	-2.20972
O	-2.40142	-5.45547	0.94225
O	-2.74863	-4.28137	-3.44816

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1788.9469493
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.445979
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1790.8162856
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1787.548257
Number of imaginary frequencies: 0

2 + NMN (reactants - endo)

Re	0.31335	0.03508	-0.73915
C	-1.56106	0.87498	0.06008
C	-1.62028	-0.57762	0.14104
C	-2.63439	-1.25735	-0.64386
C	-3.41757	-0.59028	-1.53639
C	-3.33297	0.83931	-1.64710
C	-2.48568	1.53814	-0.84412
N	0.63393	-2.11839	-0.67152
C	0.00281	-3.13605	-1.25208
C	0.65088	-4.34228	-0.94840
C	1.72152	-3.96577	-0.15608
N	1.68696	-2.62742	-0.00423
N	1.07321	-0.00560	1.42644
C	0.69486	0.57392	2.56792
C	1.48426	0.11155	3.63162
C	2.35727	-0.78868	3.04202
N	2.08666	-0.83587	1.72542
N	2.44517	-0.04980	-1.22187
C	3.16874	0.58298	-2.14444
C	4.52426	0.25688	-1.99686
C	4.54924	-0.62505	-0.92698
N	3.29062	-0.78415	-0.48079
B	2.74514	-1.70695	0.63470
N	0.71561	2.17385	-0.83696
C	0.29463	3.06375	-1.79403
C	0.84530	4.28931	-1.53604
N	1.61246	4.13562	-0.40506
C	1.50458	2.84572	-0.02054
C	2.39216	5.16199	0.25202
C	-0.25930	-0.00928	-2.50463
O	-0.61672	-0.02807	-3.61998
H	-1.30269	1.45739	0.94967

H	-1.35471	-1.06542	1.08493
H	-2.78317	-2.32819	-0.48229
H	-4.15214	-1.13268	-2.13616
H	-3.99327	1.36380	-2.34165
H	-2.49443	2.63211	-0.86166
H	-0.87689	-2.94576	-1.86177
H	0.37869	-5.34373	-1.26787
H	2.51171	-4.55216	0.30603
H	-0.14158	1.27029	2.59947
H	1.41668	0.39035	4.67901
H	3.14976	-1.40120	3.46509
H	2.67587	1.22971	-2.86730
H	5.36275	0.59915	-2.59609
H	5.37238	-1.15840	-0.45793
H	3.64531	-2.36295	1.11626
H	-0.37079	2.75298	-2.59516
H	0.76053	5.24142	-2.05201
H	2.01177	2.42784	0.84647
H	2.89516	4.72627	1.12361
H	1.74311	5.98061	0.59265
H	3.15398	5.56346	-0.43057
C	-3.20188	0.71189	2.83461
C	-4.30553	0.93893	1.84425
C	-4.83120	-0.24247	1.51711
C	-4.11497	-1.31370	2.28607
H	-4.55924	1.93011	1.47564
H	-5.62901	-0.47178	0.81457
N	-3.16730	-0.65370	3.07063
C	-2.19850	-1.31591	3.90718
H	-2.51318	-2.36082	4.02012
H	-1.19514	-1.28656	3.45462
H	-2.15339	-0.83094	4.89176
O	-4.29380	-2.50278	2.26365
O	-2.46696	1.52689	3.33910

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1788.9535865
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.447891
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1790.8220136
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1787.548257
Number of imaginary frequencies: 0

2 + NMN (Transition state - exo)

Re	-0.05722	0.99541	-0.44944
C	-0.26114	-1.17135	-0.31055
C	-0.34891	-0.76828	-1.70516
C	-1.60444	-1.13148	-2.36961
C	-2.80521	-1.18405	-1.63333
C	-2.72501	-1.55243	-0.30552
C	-1.44888	-1.85703	0.21026
N	0.01107	1.93762	-2.41222
C	-0.87270	1.99281	-3.40564
C	-0.36482	2.76406	-4.46057
C	0.88100	3.17301	-4.01676
N	1.08222	2.66156	-2.78688
N	2.18380	0.65305	-0.77542
C	3.02568	-0.35013	-0.52309
C	4.31616	-0.02926	-0.96739
C	4.18091	1.24004	-1.50730
N	2.89730	1.61917	-1.37668
N	0.60918	3.01740	0.10100
C	0.21969	3.83916	1.07475
C	1.00105	5.00275	1.06034
C	1.87303	4.81589	-0.00208
N	1.61801	3.61594	-0.55229
B	2.23376	2.94674	-1.80414
N	0.23207	0.68484	1.68858
C	-0.72079	0.37705	2.62792
C	-0.13502	0.34880	3.86341
N	1.19318	0.64638	3.66639
C	1.36752	0.84162	2.34201
C	2.21359	0.74247	4.68814
C	-1.85143	1.41212	-0.20477
O	-2.96450	1.72390	-0.02348
H	0.67678	-1.61146	0.04904
H	0.54217	-0.88626	-2.33399
H	-1.66564	-1.01244	-3.45473
H	-3.76862	-1.12357	-2.14317
H	-3.62330	-1.79100	0.26729
H	-1.38622	-2.30875	1.20430
H	-1.82715	1.48173	-3.30726
H	-0.84276	2.99382	-5.40807
H	1.63813	3.79740	-4.48436
H	2.67091	-1.25736	-0.03913
H	5.21373	-0.63801	-0.91161
H	4.90675	1.89890	-1.97752
H	-0.60514	3.55422	1.72475
H	0.92751	5.86506	1.71628
H	2.64983	5.45703	-0.41151

H	3.05825	3.67743	-2.31155
H	-1.75552	0.20458	2.34476
H	-0.54261	0.14691	4.84982
H	2.32172	1.10252	1.88906
H	3.17239	0.98590	4.21490
H	2.31538	-0.21282	5.22129
H	1.96444	1.53431	5.40807
C	-2.48546	-3.80421	-2.85785
C	-1.18891	-3.30439	-2.32532
C	-1.10691	-3.67422	-0.98010
C	-2.34910	-4.41839	-0.63442
H	-0.34548	-3.17372	-2.99989
H	-0.18755	-3.88609	-0.43815
N	-3.15705	-4.36829	-1.76947
C	-4.49471	-4.89508	-1.82831
H	-4.53653	-5.86506	-1.31444
H	-5.21373	-4.21392	-1.34664
H	-4.76563	-5.01385	-2.88520
O	-2.65530	-4.96061	0.40146
O	-2.92349	-3.75038	-3.98234

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1788.9186223
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP : 0.451132
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1790.7843588
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1787.516145
Number of imaginary frequencies: 1

2 + NMN (Transition state - endo)

Re	0.69115	-0.06714	-0.40776
C	-1.10461	0.68183	0.56661
C	-1.16068	-0.77325	0.51444
C	-2.31352	-1.31262	-0.20594
C	-2.86641	-0.59573	-1.29150
C	-2.80819	0.77983	-1.24478
C	-2.20187	1.36809	-0.11295
N	1.04311	-2.21508	-0.47428
C	0.37332	-3.21106	-1.04865
C	1.03441	-4.42745	-0.82772
C	2.15193	-4.07995	-0.08824
N	2.13116	-2.74796	0.11112
N	1.57662	-0.20014	1.70322
C	1.28360	0.35259	2.88176
C	2.13677	-0.14250	3.87820
C	2.96015	-1.03273	3.20694
N	2.60168	-1.04296	1.91102
N	2.80442	-0.09857	-1.00048

C	3.47398	0.58875	-1.92477
C	4.83714	0.26802	-1.86584
C	4.92405	-0.66939	-0.84723
N	3.69226	-0.86362	-0.34462
B	3.21160	-1.85201	0.74521
N	1.06469	2.08033	-0.40045
C	0.50410	3.03005	-1.21788
C	1.04599	4.24988	-0.91974
N	1.95035	4.03168	0.09296
C	1.92793	2.71126	0.37222
C	2.76824	5.03129	0.74574
C	0.07463	-0.01159	-2.15869
O	-0.26882	0.03823	-3.27704
H	-0.81474	1.17362	1.49923
H	-0.87988	-1.34604	1.40592
H	-2.49381	-2.38839	-0.13129
H	-3.47405	-1.10774	-2.04081
H	-3.36973	1.39046	-1.95522
H	-2.28189	2.44879	0.03326
H	-0.54339	-2.99980	-1.59335
H	0.73940	-5.41711	-1.16301
H	2.96491	-4.68358	0.30725
H	0.47442	1.07481	2.97063
H	2.14547	0.10801	4.93486
H	3.77450	-1.66048	3.56022
H	2.93919	1.26784	-2.58561
H	5.64080	0.64928	-2.48876
H	5.77442	-1.21943	-0.45175
H	4.14023	-2.52115	1.14673
H	-0.24370	2.76262	-1.95939
H	0.86933	5.23832	-1.33401
H	2.54869	2.24256	1.13282
H	3.39772	4.54247	1.49891
H	2.13693	5.77928	1.24504
H	3.41759	5.53342	0.01540
C	-3.10704	1.05574	2.58550
C	-3.79338	0.73830	1.30062
C	-3.89180	-0.65554	1.20572
C	-3.30282	-1.23760	2.44280
H	-4.50862	1.45068	0.89606
H	-4.68574	-1.19777	0.69745
N	-2.80155	-0.16614	3.18242
C	-2.02605	-0.32147	4.38374
H	-2.56531	-0.94528	5.11030
H	-1.05590	-0.79758	4.17050
H	-1.86040	0.67854	4.80510

O	-3.22200	-2.39295	2.78401
O	-2.81708	2.13510	3.04930

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1788.9200786
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.452815
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1790.785063
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1787.516363
Number of imaginary frequencies: 1

2 + NMN (Product - exo)

Re	0.08314	0.63133	0.11835
C	-0.11016	-1.51493	0.25738
C	-0.19383	-1.11479	-1.12436
C	-1.46617	-1.66453	-1.79593
C	-2.68759	-1.32690	-0.98618
C	-2.61419	-1.69090	0.29722
C	-1.32445	-2.36466	0.67778
N	0.16572	1.57216	-1.84574
C	-0.69963	1.59407	-2.85619
C	-0.18372	2.35211	-3.91677
C	1.04859	2.78612	-3.45914
N	1.23391	2.30188	-2.21581
N	2.32766	0.30024	-0.20233
C	3.17083	-0.69808	0.06159
C	4.46602	-0.36966	-0.36404
C	4.33155	0.89891	-0.90566
N	3.04399	1.27114	-0.79302
N	0.75075	2.67295	0.66650
C	0.35123	3.49965	1.63160
C	1.12695	4.66725	1.61367
C	2.00587	4.47731	0.55744
N	1.75984	3.27191	0.01507
B	2.38078	2.59600	-1.22989
N	0.39449	0.33290	2.25544
C	-0.53006	-0.05221	3.19388
C	0.06556	-0.07074	4.42467
N	1.37173	0.31162	4.22534
C	1.52315	0.54466	2.90406
C	2.39286	0.44750	5.24150
C	-1.69448	1.10194	0.38448
O	-2.77550	1.50074	0.59686
H	0.82010	-1.97079	0.62413
H	0.69210	-1.24254	-1.76219
H	-1.55590	-1.36745	-2.84887
H	-3.54298	-0.80261	-1.41603

H	-3.40458	-1.49637	1.02449
H	-1.29408	-2.65828	1.73561
H	-1.64691	1.06909	-2.76594
H	-0.64729	2.55628	-4.87716
H	1.80673	3.40982	-3.92599
H	2.81148	-1.60707	0.53855
H	5.36614	-0.97347	-0.29618
H	5.06013	1.56171	-1.36607
H	-0.47744	3.21587	2.27732
H	1.04523	5.53395	2.26288
H	2.78153	5.11952	0.14743
H	3.20637	3.32462	-1.73897
H	-1.55415	-0.28126	2.91351
H	-0.32113	-0.31869	5.40896
H	2.45676	0.87018	2.45008
H	3.33120	0.75839	4.76670
H	2.55685	-0.51097	5.75311
H	2.10285	1.20735	5.98040
C	-2.48077	-3.97359	-2.26172
C	-1.29081	-3.21541	-1.70433
C	-1.20698	-3.63419	-0.22569
C	-2.35465	-4.60560	-0.02696
H	-0.39921	-3.50710	-2.27925
H	-0.26925	-4.15817	0.01333
N	-3.01738	-4.74739	-1.23777
C	-4.19523	-5.56605	-1.39140
H	-4.00161	-6.58013	-1.01630
H	-5.03780	-5.14109	-0.82644
H	-4.44621	-5.59551	-2.45869
O	-2.67524	-5.17051	0.98922
O	-2.91668	-3.93145	-3.38465

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1788.9871695
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.456956
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1790.8486142
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1787.575836
Number of imaginary frequencies: 0

2 + NMN (Product - endo)

Re	0.28581	-0.04782	-0.65188
C	-1.45773	0.67900	0.38297
C	-1.49172	-0.76148	0.34751
C	-2.82402	-1.27977	-0.22361
C	-3.12804	-0.62394	-1.54375
C	-3.09601	0.71096	-1.51411

C	-2.75602	1.29389	-0.16880
N	0.65982	-2.19225	-0.74707
C	-0.04462	-3.19345	-1.26808
C	0.63063	-4.40750	-1.08007
C	1.79200	-4.05318	-0.41499
N	1.78253	-2.71953	-0.22631
N	1.26623	-0.21140	1.41735
C	1.00564	0.30494	2.61926
C	1.91320	-0.18609	3.56866
C	2.73209	-1.03807	2.84454
N	2.32128	-1.02998	1.56397
N	2.38898	-0.06188	-1.34446
C	3.00745	0.63421	-2.29690
C	4.37447	0.32329	-2.30619
C	4.51747	-0.61852	-1.29794
N	3.31267	-0.82297	-0.73706
B	2.88702	-1.82179	0.36422
N	0.67333	2.09759	-0.62698
C	0.05403	3.07074	-1.37026
C	0.61278	4.28262	-1.07150
N	1.58749	4.03535	-0.13334
C	1.58759	2.70613	0.10291
C	2.44902	5.01607	0.49098
C	-0.35050	0.02632	-2.39450
O	-0.65347	0.08926	-3.52533
H	-1.15281	1.19321	1.30272
H	-1.18029	-1.32478	1.23779
H	-2.86251	-2.37633	-0.26268
H	-3.31227	-1.20240	-2.45098
H	-3.25290	1.33650	-2.39492
H	-2.72949	2.39183	-0.16626
H	-0.99547	-2.98721	-1.75221
H	0.31589	-5.40008	-1.38756
H	2.62812	-4.65311	-0.06480
H	0.17777	0.99790	2.75401
H	1.95904	0.04086	4.62969
H	3.57550	-1.65213	3.15052
H	2.43593	1.31113	-2.92872
H	5.14410	0.71307	-2.96578
H	5.38960	-1.16499	-0.94739
H	3.83603	-2.48910	0.71888
H	-0.74241	2.82455	-2.06665
H	0.40388	5.28336	-1.43842
H	2.26044	2.21521	0.80281
H	3.12676	4.50607	1.18601
H	1.85400	5.74947	1.05263

H	3.04893	5.53913	-0.26653
C	-3.55598	1.12729	2.25231
C	-3.86899	0.78604	0.80599
C	-3.92045	-0.75303	0.76174
C	-3.66676	-1.19483	2.19042
H	-4.83258	1.24887	0.54649
H	-4.90473	-1.13563	0.45504
N	-3.46684	-0.05954	2.96727
C	-3.11667	-0.12593	4.36457
H	-3.80530	-0.79903	4.89235
H	-2.09291	-0.51116	4.48813
H	-3.18044	0.88825	4.77745
O	-3.62387	-2.31920	2.62175
O	-3.38957	2.22340	2.72952

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1788.9890515
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.456631
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1790.8497391
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1787.577057
Number of imaginary frequencies: 0

3 + NMN (reactants - endo)

Os	-1.39933	-0.58486	0.11246
N	-1.84104	1.56298	-0.02566
H	-2.27349	1.97494	0.80620
H	-0.99373	2.12330	-0.17403
N	-3.55490	-1.04612	0.27330
H	-4.06960	-0.39656	0.87541
H	-4.06321	-1.01077	-0.61489
N	-1.64661	-0.80750	-2.06081
H	-1.50495	0.05685	-2.59230
H	-0.95066	-1.45295	-2.44726
N	-1.45261	-0.49526	2.30681
H	-0.71543	-1.07571	2.71977
H	-1.27901	0.43596	2.69737
N	-0.93457	-2.71161	0.23316
H	0.02123	-2.87715	-0.10503
H	-0.94350	-3.11101	1.17541
C	0.71970	0.07335	0.68079
C	1.52839	-0.85761	1.42889
C	2.18038	-1.88355	0.80222
C	2.12930	-2.00644	-0.62206
C	1.42756	-1.09762	-1.36769
C	0.66685	-0.05063	-0.73288
H	0.56058	1.04770	1.15360

H	2.80917	-2.56737	1.37645
H	2.72340	-2.77896	-1.11545
H	0.46216	0.82673	-1.35440
H	-2.46350	1.83120	-0.79315
H	-2.54853	-1.16895	-2.38365
H	-3.76506	-1.97559	0.65006
H	-2.32045	-0.80996	2.74963
H	-1.52746	-3.33580	-0.32061
C	3.02299	2.23661	0.82290
C	4.15171	1.34174	0.39950
C	4.11297	1.20812	-0.92862
C	2.95674	2.00774	-1.45588
H	4.84427	0.90199	1.11568
O	2.62707	2.48357	1.93228
O	2.49585	2.03194	-2.56728
H	4.76572	0.63073	-1.58169
N	2.41374	2.66862	-0.35460
C	1.29865	3.57498	-0.41347
H	0.66699	3.31235	-1.27676
H	0.74336	3.51914	0.53571
H	1.62393	4.61724	-0.54716
H	1.68438	-0.68388	2.49715
H	1.50377	-1.11049	-2.45834

Electronic energy (a.u.) at ωB97xd/def2-SVP: –1003.1912797
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.344602
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1004.224452
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1002.641361
Number of imaginary frequencies: 0

3 + NMN (Transition state - endo)

Os	0.08219	0.39474	-0.09964
N	-0.52830	2.50625	-0.22301
H	-0.82028	2.92216	0.66620
H	0.22900	3.11673	-0.55010
N	-2.04592	-0.23984	0.06826
H	-2.55306	0.23056	0.82363
H	-2.60843	-0.03788	-0.76335
N	-0.18722	0.15432	-2.26807
H	-0.17347	1.03197	-2.79613
H	0.57888	-0.39149	-2.67446
N	0.05038	0.44647	2.09564
H	0.85255	-0.06116	2.48204
H	0.13375	1.38312	2.50225
N	0.63347	-1.70522	0.01591

H	1.65834	-1.78216	-0.03207
H	0.36803	-2.19212	0.87645
C	2.08038	1.26784	0.44386
C	3.13614	0.52178	1.12257
C	3.57207	-0.71438	0.58136
C	3.52313	-0.85975	-0.79011
C	3.03792	0.23798	-1.54604
C	2.02714	1.11618	-0.96417
H	1.83793	2.23207	0.90344
H	4.11632	-1.42892	1.20363
H	4.02976	-1.69118	-1.28632
H	1.74610	1.96358	-1.59914
H	-1.30609	2.69990	-0.86018
H	-1.04169	-0.32231	-2.57011
H	-2.18952	-1.23983	0.23967
H	-0.77049	0.03371	2.54772
H	0.28144	-2.30066	-0.73871
C	4.26149	3.09457	0.62538
C	4.77536	1.72144	0.28704
C	4.72091	1.58008	-1.09985
C	4.16742	2.85868	-1.66776
H	5.51291	1.25445	0.93805
O	4.09106	3.57942	1.71216
O	3.90575	3.10916	-2.81422
H	5.41067	0.98787	-1.69939
N	3.91774	3.69444	-0.58212
C	3.34207	5.01615	-0.68727
H	3.41997	5.34362	-1.73114
H	2.28262	5.02024	-0.38141
H	3.88736	5.71095	-0.03607
H	3.31170	0.73534	2.18073
H	3.13420	0.22272	-2.63530

Electronic energy (a.u.) at ωB97xd/def2-SVP: -1003.1468246
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.347517
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1004.175393
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP:
Number of imaginary frequencies: 1

3 + NMN (Product - endo)

Os	-1.34672	-0.63707	0.10958
N	-2.05893	1.44314	0.01154
H	-2.31876	1.85057	0.91455
H	-1.34621	2.08280	-0.35795
N	-3.46853	-1.38218	0.28749
H	-3.98718	-0.94514	1.05492

H	-4.04734	-1.18773	-0.53459
N	-1.64790	-0.86766	-2.05500
H	-1.68336	0.01848	-2.56731
H	-0.86685	-1.37059	-2.48579
N	-1.38412	-0.62295	2.30447
H	-0.57660	-1.12219	2.68851
H	-1.31526	0.31057	2.72043
N	-0.76757	-2.73208	0.19984
H	0.25947	-2.77408	0.19675
H	-1.06411	-3.24516	1.03465
C	0.53744	0.34719	0.64730
C	1.81069	-0.24331	1.26837
C	2.07663	-1.64933	0.79472
C	2.04339	-1.79762	-0.53654
C	1.73830	-0.53177	-1.29561
C	0.49468	0.18631	-0.75054
H	0.25801	1.30315	1.10853
H	2.36383	-2.44268	1.48994
H	2.30197	-2.72536	-1.05421
H	0.18464	1.01736	-1.39785
H	-2.87844	1.59827	-0.58228
H	-2.48663	-1.37772	-2.34643
H	-3.57149	-2.38989	0.44219
H	-2.20055	-1.05348	2.74803
H	-1.07174	-3.31303	-0.58622
C	2.75804	2.10996	0.84752
C	2.94934	0.61580	0.61280
C	2.90308	0.44803	-0.91168
C	2.68067	1.85497	-1.45561
H	3.91364	0.31849	1.04812
O	2.60179	2.65360	1.90777
O	2.44914	2.14688	-2.59820
H	3.84390	0.06269	-1.32920
N	2.71495	2.74099	-0.38704
C	2.57703	4.17838	-0.53029
H	2.38904	4.39761	-1.58790
H	1.74856	4.54199	0.09245
H	3.49857	4.68128	-0.20830
H	1.84421	-0.13027	2.35942
H	1.70976	-0.66600	-2.38422

Electronic energy (a.u.) at ωB97xd/def2-SVP: –1003.2124487
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.353316
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1004.237046
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1002.662696

Number of imaginary frequencies: 0

Benzene + NMN (reactants)

C	1.60041	0.26362	-0.91957
C	1.38243	-1.07396	-1.24939
C	0.48773	-1.40228	-2.26932
C	-0.18453	-0.39399	-2.96018
C	0.02776	0.94269	-2.62324
C	0.91888	1.27241	-1.60085
H	2.29993	0.52316	-0.12154
H	1.90173	-1.86451	-0.70377
H	0.31793	-2.45005	-2.52735
H	-0.87993	-0.65158	-3.76236
H	-0.50193	1.73318	-3.15982
H	1.07658	2.31781	-1.32787
C	-0.83125	1.14543	1.20077
C	-1.78030	0.47086	0.25142
C	-1.62235	-0.84883	0.35604
C	-0.55846	-1.12351	1.38095
H	-2.44860	1.03713	-0.39413
H	-2.12676	-1.64884	-0.18212
N	-0.15154	0.11982	1.85319
C	0.90216	0.31553	2.81573
H	0.64581	-0.14992	3.77790
H	1.84421	-0.12355	2.45533
H	1.02916	1.39661	2.95406
O	-0.11863	-2.18365	1.74173
O	-0.66587	2.32357	1.38014

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-630.3392824
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.157753
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -631.0299041
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -629.9308415
Number of imaginary frequencies: 0

Benzene + NMN (Transition state)

C	-1.18025	0.60954	0.37378
C	-1.23848	-0.75107	0.35304
C	-2.40562	-1.34271	-0.23347
C	-3.01654	-0.64796	-1.33443
C	-2.95853	0.70997	-1.31365
C	-2.29173	1.31617	-0.19308
H	-0.40656	1.15152	0.92041
H	-0.51472	-1.37363	0.88201
H	-2.51533	-2.42832	-0.17348
H	-3.60554	-1.19584	-2.07242

H	-3.49774	1.32836	-2.03375
H	-2.30903	2.40479	-0.09942
C	-3.07265	1.13133	2.51250
C	-3.75636	0.72699	1.24385
C	-3.81510	-0.67742	1.22183
C	-3.16900	-1.17530	2.47725
H	-4.52629	1.38307	0.84178
H	-4.63758	-1.25336	0.80142
N	-2.68378	-0.05078	3.14088
C	-1.90279	-0.10615	4.35079
H	-2.29218	-0.90055	5.00081
H	-0.84449	-0.31763	4.13261
H	-1.97780	0.86697	4.85207
O	-3.05090	-2.30918	2.86838
O	-2.86270	2.24026	2.93536

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-630.2863335
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.161982
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -630.9730492
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -629.8809221
Number of imaginary frequencies: 1

Benzene + NMN (Product)

C	1.52132	0.63835	-1.16809
C	1.47783	-0.69544	-1.19173
C	0.09707	-1.26025	-1.47245
C	-0.45154	-0.60510	-2.72818
C	-0.40820	0.72829	-2.70448
C	0.18051	1.30143	-1.42704
H	2.41255	1.22598	-0.94287
H	2.32872	-1.34741	-0.98864
H	0.07845	-2.35557	-1.50335
H	-0.86053	-1.19793	-3.54791
H	-0.77689	1.37519	-3.50214
H	0.23314	2.39604	-1.41907
C	-0.25396	1.15316	1.09764
C	-0.77075	0.79696	-0.28654
C	-0.82075	-0.73579	-0.31385
C	-0.32933	-1.17013	1.05695
H	-1.76024	1.25871	-0.41270
H	-1.83821	-1.12684	-0.45542
N	-0.05313	-0.02989	1.79837
C	0.47363	-0.08196	3.14200
H	-0.16526	-0.71514	3.77194
H	1.48979	-0.50214	3.14187
H	0.49873	0.94241	3.53263

O	-0.18231	-2.29499	1.46036
O	-0.03909	2.25503	1.53261

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-630.3419725
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.167886
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -631.024834
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -629.9312066
Number of imaginary frequencies: 0

7' + NMN (reactants - exo)

W	-0.46131	-0.51424	0.77062
P	1.08063	-2.47219	1.07331
O	1.41370	1.10216	2.38609
N	-2.27991	0.81886	0.92373
N	-3.51219	0.30687	1.10267
N	-1.97625	-1.88206	-0.34537
N	-3.23321	-1.99806	0.11498
N	-1.54285	-1.25221	2.58698
N	-2.85000	-1.56573	2.57657
N	0.64861	0.47273	1.72254
C	2.14093	-0.04590	-1.11227
H	2.91680	-0.79536	-1.29953
C	0.75565	-0.44106	-1.16153
H	0.54663	-1.31811	-1.78390
C	-0.24738	0.63318	-1.13816
C	0.22482	1.99035	-1.07723
C	3.92215	1.60256	-0.64836
H	4.67223	0.80852	-0.67951
C	1.99075	3.66053	-0.62200
H	1.24524	4.45908	-0.63097
C	2.53657	1.24307	-0.82896
C	1.54186	2.30415	-0.81569
C	4.28967	2.89373	-0.44248
C	3.30532	3.94364	-0.42885
C	-4.40606	1.30483	1.24075
H	-5.45845	1.08397	1.40117
C	-3.73215	2.51093	1.14980
H	-4.14646	3.51223	1.21860
C	-2.39256	2.14452	0.95652
H	-1.50567	2.76449	0.85066
C	-3.94008	-2.83057	-0.66724
H	-4.98352	-3.04211	-0.44733
C	-3.11362	-3.28079	-1.68548
H	-3.36126	-3.96197	-2.49392
C	-1.89028	-2.64937	-1.43409
H	-0.96018	-2.70899	-1.99412

C	-3.25206	-1.88913	3.81893
H	-4.28841	-2.15561	4.01126
C	-2.16510	-1.78490	4.67299
H	-2.13836	-1.97035	5.74249
C	-1.11620	-1.36571	3.84469
H	-0.08438	-1.12217	4.09107
C	2.69406	-1.97487	1.77244
H	3.35445	-2.83892	1.93617
H	2.52479	-1.44375	2.71962
H	3.17030	-1.25909	1.08812
C	1.55624	-3.51382	-0.36431
H	2.05139	-2.90930	-1.13486
H	0.65546	-3.97170	-0.79757
H	2.24063	-4.31466	-0.04775
C	0.50566	-3.78402	2.22607
H	-0.48556	-4.13525	1.90293
H	0.40411	-3.38322	3.24220
H	1.20657	-4.63165	2.24336
B	-3.71573	-1.20418	1.34595
H	-4.88283	-1.44956	1.56326
H	-1.18262	0.47288	-1.68779
H	5.34184	3.14702	-0.29400
H	3.62680	4.97518	-0.26888
C	3.21605	1.29454	-3.94329
C	1.83507	0.71924	-4.03739
C	0.95172	1.72238	-4.02636
C	1.70162	3.01708	-3.92896
H	1.65980	-0.35145	-4.11274
O	4.27168	0.71296	-3.93284
O	1.26337	4.13886	-3.90896
H	-0.13352	1.68596	-4.08850
N	3.04966	2.67397	-3.87731
C	4.12904	3.62493	-3.80497
H	4.98222	3.14468	-3.31032
H	4.43393	3.96467	-4.80722
H	3.79846	4.48925	-3.21559
H	-0.48755	2.80419	-1.23808

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2143.4281691
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.503657
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2145.4459093
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2141.679212
Number of imaginary frequencies: 0

7' + NMN (reactants - endo)

W	-0.02511	-0.31985	0.85072

P	1.77312	-2.04725	1.14767
O	1.47781	1.47615	2.65599
N	-2.04260	0.69303	0.93179
N	-3.18101	-0.02186	1.00469
N	-1.22983	-1.82006	-0.46466
N	-2.47088	-2.17704	-0.08897
N	-1.07905	-1.33193	2.54509
N	-2.31036	-1.85597	2.42035
N	0.85795	0.77223	1.91840
C	2.56468	0.63745	-0.86409
H	3.45685	0.01511	-0.99301
C	1.26766	0.01921	-0.97860
H	1.24516	-0.86610	-1.61803
C	0.10043	0.91856	-0.99771
C	0.33551	2.33313	-0.92259
C	4.04019	2.57398	-0.44405
H	4.91036	1.91199	-0.41480
C	1.79848	4.28371	-0.51849
H	0.92896	4.94580	-0.54916
C	2.73542	1.98065	-0.62044
C	1.57922	2.86432	-0.65763
C	4.19208	3.91695	-0.31180
C	3.04738	4.79105	-0.35056
C	-4.23626	0.80871	1.10407
H	-5.24547	0.41119	1.17828
C	-3.76884	2.11223	1.09710
H	-4.34870	3.02790	1.16200
C	-2.37703	1.97979	0.99192
H	-1.60115	2.74105	0.96455
C	-3.00720	-3.01354	-0.99353
H	-4.01289	-3.40311	-0.85626
C	-2.08131	-3.21398	-2.00536
H	-2.18432	-3.82819	-2.89476
C	-0.98113	-2.43633	-1.62380
H	-0.04741	-2.27770	-2.16121
C	-2.72976	-2.32430	3.60968
H	-3.71604	-2.77069	3.70972
C	-1.73262	-2.09940	4.54620
H	-1.74275	-2.34951	5.60273
C	-0.71967	-1.45763	3.82232
H	0.23911	-1.06545	4.15643
C	3.26379	-1.36373	1.95427
H	4.04309	-2.12703	2.09475
H	2.97686	-0.93479	2.92472
H	3.64936	-0.53620	1.34295
C	2.44565	-2.92726	-0.31802

H	2.89350	-2.22350	-1.03096
H	1.62954	-3.46008	-0.82676
H	3.20845	-3.65736	-0.00996
C	1.34750	-3.48923	2.20582
H	0.42798	-3.95568	1.82225
H	1.15546	-3.16564	3.23627
H	2.15989	-4.23089	2.20895
B	-3.14589	-1.55981	1.15239
H	-4.26798	-2.00247	1.27464
H	-0.77645	0.61632	-1.58065
H	5.18669	4.34672	-0.17311
H	3.19401	5.86780	-0.24080
C	-0.04053	2.15111	-4.09042
C	1.42544	2.38434	-3.88077
C	2.05294	1.20556	-3.91604
C	1.03035	0.12738	-4.11356
H	1.83839	3.37899	-3.72598
O	-0.93598	2.95399	-4.12570
O	1.19121	-1.07061	-4.13121
H	3.11206	0.98899	-3.79960
N	-0.19004	0.77066	-4.24889
C	-1.45719	0.09874	-4.38281
H	-1.42676	-0.61216	-5.21978
H	-1.71639	-0.45129	-3.46440
H	-2.22097	0.86321	-4.57234
H	-0.50014	3.01186	-1.11386

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2143.4308494
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.504392
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2145.4484644
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2141.680306
Number of imaginary frequencies: 0

7' + NMN (Transition state - exo)

W	-0.35026	-0.62460	0.09698
P	1.22109	-2.56508	0.41253
O	1.52475	0.99126	1.70965
N	-2.17611	0.69205	0.26610
N	-3.39487	0.17934	0.51761
N	-1.89502	-2.03892	-0.91282
N	-3.13106	-2.15398	-0.39718
N	-1.36118	-1.31100	1.97997
N	-2.66448	-1.63519	2.03287
N	0.76904	0.37536	1.02300
C	2.16870	-0.20148	-1.96805

H	2.93970	-0.94618	-2.18950
C	0.78642	-0.62790	-1.85153
H	0.54116	-1.49678	-2.47298
C	-0.20442	0.46256	-1.82323
C	0.33133	1.80351	-1.90442
C	3.94049	1.33406	-1.11625
H	4.68240	0.53380	-1.16652
C	2.04760	3.41027	-1.07293
H	1.31619	4.22108	-1.08529
C	2.58801	1.04158	-1.44724
C	1.62473	2.09765	-1.42324
C	4.30584	2.60039	-0.73806
C	3.34997	3.65045	-0.71891
C	-4.29693	1.17367	0.61744
H	-5.34112	0.95216	0.82390
C	-3.64230	2.37897	0.42487
H	-4.06771	3.37781	0.43990
C	-2.30553	2.01569	0.21171
H	-1.43232	2.63778	0.03086
C	-3.85832	-3.01963	-1.12244
H	-4.88935	-3.23524	-0.85340
C	-3.06863	-3.49393	-2.15865
H	-3.34057	-4.20351	-2.93414
C	-1.84435	-2.84085	-1.97894
H	-0.93777	-2.90888	-2.57522
C	-3.01565	-1.90791	3.30216
H	-4.04150	-2.17328	3.54582
C	-1.89768	-1.75897	4.10863
H	-1.82848	-1.89831	5.18318
C	-0.88560	-1.36624	3.22396
H	0.15116	-1.09889	3.42066
C	2.87513	-2.02367	0.96848
H	3.53349	-2.87828	1.18179
H	2.76449	-1.39583	1.86390
H	3.32300	-1.39100	0.19049
C	1.59824	-3.67701	-0.99872
H	2.02719	-3.10783	-1.83327
H	0.67357	-4.16448	-1.33925
H	2.31467	-4.45345	-0.69280
C	0.73904	-3.80829	1.67731
H	-0.27499	-4.17309	1.45683
H	0.72261	-3.35179	2.67469
H	1.44006	-4.65594	1.68394
B	-3.57693	-1.32354	0.82357
H	-4.73335	-1.56937	1.09057
H	-1.14063	0.30252	-2.37229

H	5.34112	2.80955	-0.45984
H	3.66018	4.65594	-0.42698
C	3.30088	1.13370	-4.27816
C	1.94193	0.53534	-4.17821
C	1.02083	1.56449	-4.16718
C	1.76047	2.85010	-4.24470
H	1.76601	-0.49701	-4.47086
O	4.37504	0.58324	-4.34964
O	1.32914	3.97863	-4.28026
H	-0.03255	1.50903	-4.42938
N	3.11644	2.51326	-4.24622
C	4.19181	3.46879	-4.22834
H	4.89323	3.22926	-3.41699
H	4.73891	3.46898	-5.18318
H	3.75240	4.45961	-4.05791
H	-0.35223	2.63616	-2.09073

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2143.4172243
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.506790
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2145.4317916
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2141.669989
Number of imaginary frequencies: 1

7' + NMN (Transition state - endo)

W	-0.00949	-0.97357	0.69536
P	1.81008	-2.70696	0.87722
O	1.61811	0.76050	2.44986
N	-2.00304	0.05852	0.91750
N	-3.14085	-0.63790	1.09396
N	-1.31781	-2.50466	-0.46809
N	-2.53901	-2.82374	-0.00486
N	-0.93966	-1.94960	2.48634
N	-2.18442	-2.45683	2.47302
N	0.95361	0.09808	1.71260
C	2.42993	-0.08837	-1.31432
H	3.28109	-0.72517	-1.57330
C	1.12195	-0.69898	-1.21709
H	0.99904	-1.56497	-1.87239
C	-0.00967	0.25247	-1.14289
C	0.34387	1.64826	-1.15029
C	3.98470	1.62369	-0.37125
H	4.82600	0.92947	-0.45024
C	1.83450	3.41600	-0.20858
H	0.99711	4.11679	-0.15788
C	2.68450	1.17248	-0.72071

C	1.59174	2.08577	-0.64204
C	4.18399	2.90671	0.07587
C	3.09642	3.81296	0.15935
C	-4.17747	0.20894	1.23486
H	-5.18367	-0.17226	1.39044
C	-3.69793	1.50552	1.14829
H	-4.26256	2.43025	1.21781
C	-2.31917	1.35104	0.95118
H	-1.54030	2.10121	0.83841
C	-3.13271	-3.70342	-0.82826
H	-4.13249	-4.07249	-0.61351
C	-2.26618	-3.97541	-1.87585
H	-2.42605	-4.63949	-2.71983
C	-1.13990	-3.19278	-1.59866
H	-0.22049	-3.09388	-2.17132
C	-2.51383	-2.88807	3.70353
H	-3.49531	-3.31547	3.89361
C	-1.44200	-2.65605	4.55204
H	-1.37145	-2.87982	5.61215
C	-0.48159	-2.04808	3.73407
H	0.50364	-1.65736	3.98216
C	3.38290	-1.98817	1.46791
H	4.15085	-2.76040	1.62056
H	3.19686	-1.44608	2.40591
H	3.73633	-1.24865	0.73757
C	2.30326	-3.66898	-0.60683
H	2.57536	-3.01292	-1.44431
H	1.46028	-4.30107	-0.92123
H	3.15818	-4.31898	-0.36923
C	1.51664	-4.08152	2.06109
H	0.55317	-4.55876	1.82929
H	1.46448	-3.69781	3.08755
H	2.32007	-4.83040	1.99995
B	-3.11396	-2.17196	1.26912
H	-4.22803	-2.59781	1.48473
H	-0.92382	0.00553	-1.69592
H	5.18367	3.23557	0.36790
H	3.26825	4.83040	0.51693
C	-0.03550	1.12674	-3.96704
C	1.18612	1.74253	-3.39577
C	2.20460	0.80628	-3.44476
C	1.65227	-0.44457	-4.03368
H	1.29297	2.82164	-3.32633
O	-1.13853	1.59320	-4.12574
O	2.19910	-1.50951	-4.22135
H	3.27234	1.00855	-3.46517

N	0.30781	-0.19134	-4.28882
C	-0.63991	-1.17385	-4.74091
H	-0.07964	-2.07618	-5.01824
H	-1.36599	-1.42046	-3.94938
H	-1.19493	-0.79931	-5.61215
H	-0.45000	2.38267	-1.31039

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2143.4171354
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.507442
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2145.4319943
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2141.668384
Number of imaginary frequencies: 1

7' + NMN (Product - exo)

W	-0.39962	-0.44889	0.54676
P	1.14642	-2.41153	0.86628
O	1.41739	1.05660	2.31642
N	-2.22225	0.86494	0.73898
N	-3.43466	0.36835	1.04411
N	-1.98568	-1.87734	-0.37602
N	-3.20495	-1.98374	0.17955
N	-1.37555	-1.10025	2.48195
N	-2.67714	-1.41574	2.58470
N	0.71310	0.51822	1.51440
C	2.08391	0.02731	-1.73484
H	2.86333	-0.74910	-1.73521
C	0.68633	-0.51042	-1.39197
H	0.45217	-1.39113	-2.00573
C	-0.30268	0.55843	-1.37912
C	0.31334	1.91709	-1.72745
C	3.65134	1.35292	-0.16038
H	4.41821	0.57479	-0.19752
C	1.71881	3.37747	-0.12512
H	0.97212	4.17574	-0.13267
C	2.45864	1.19047	-0.85437
C	1.49545	2.21095	-0.84541
C	3.87178	2.52307	0.56891
C	2.90813	3.52806	0.59078
C	-4.33455	1.36738	1.10471
H	-5.37454	1.15881	1.34331
C	-3.68416	2.55938	0.82963
H	-4.10970	3.55770	0.79581
C	-2.35248	2.18286	0.60838
H	-1.48262	2.78970	0.36932
C	-3.95628	-2.85521	-0.51382
H	-4.97919	-3.06467	-0.21105

C	-3.20023	-3.34216	-1.56906
H	-3.49796	-4.05905	-2.32822
C	-1.96971	-2.68920	-1.43515
H	-1.08213	-2.75979	-2.05913
C	-2.99000	-1.64925	3.87176
H	-4.00913	-1.90075	4.15524
C	-1.84592	-1.48380	4.63770
H	-1.74347	-1.59244	5.71317
C	-0.86031	-1.12119	3.71042
H	0.18153	-0.84437	3.86590
C	2.82606	-1.89195	1.36016
H	3.44216	-2.74785	1.67205
H	2.75217	-1.15409	2.17213
H	3.29856	-1.38646	0.50838
C	1.46685	-3.55276	-0.53299
H	1.88852	-2.99906	-1.38185
H	0.52614	-4.02586	-0.84845
H	2.17444	-4.33837	-0.22984
C	0.67959	-3.61781	2.17267
H	-0.34819	-3.96610	1.99295
H	0.70369	-3.13772	3.15892
H	1.36357	-4.47935	2.17696
B	-3.61775	-1.12593	1.39404
H	-4.76932	-1.35828	1.69321
H	-1.24033	0.37632	-1.92438
H	4.80434	2.65004	1.12285
H	3.08507	4.44011	1.16474
C	3.21953	1.27392	-3.64677
C	1.93797	0.61348	-3.17312
C	0.88722	1.74108	-3.16848
C	1.63467	2.97524	-3.64063
H	1.68546	-0.19936	-3.87016
O	4.30013	0.75793	-3.78780
O	1.19248	4.08764	-3.77779
H	0.05608	1.54988	-3.86297
N	2.95681	2.61548	-3.87831
C	3.98282	3.55679	-4.25743
H	4.68744	3.70872	-3.42688
H	4.53950	3.17819	-5.12512
H	3.49282	4.50681	-4.50241
H	-0.41854	2.73618	-1.72206

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2143.5081073
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.512227
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2145.5161838
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2141.74774

Number of imaginary frequencies: 0

7' + NMN (Product - endo)

W	-0.05792	-0.20039	0.64842
P	1.74314	-1.95396	0.82891
O	1.58312	1.45917	2.45372
N	-2.03902	0.83776	0.92753
N	-3.16574	0.16388	1.22041
N	-1.45193	-1.77969	-0.34095
N	-2.63552	-2.08197	0.21994
N	-0.89879	-1.08188	2.55332
N	-2.14233	-1.58076	2.64959
N	0.93544	0.86387	1.64331
C	2.27993	0.69469	-1.66437
H	3.15212	0.02578	-1.70069
C	0.98097	-0.03907	-1.29748
H	0.85869	-0.93552	-1.91656
C	-0.14750	0.88068	-1.23610
C	0.26211	2.31805	-1.57154
C	3.66784	2.17065	-0.05331
H	4.53065	1.50120	-0.10903
C	1.47185	3.89858	0.07787
H	0.61450	4.57589	0.12363
C	2.50951	1.87899	-0.76208
C	1.41239	2.75316	-0.70499
C	3.72761	3.32483	0.73129
C	2.63292	4.18152	0.80141
C	-4.19493	1.02363	1.33319
H	-5.19243	0.66152	1.56949
C	-3.72101	2.30563	1.10644
H	-4.28256	3.23476	1.11923
C	-2.35354	2.12878	0.85650
H	-1.57993	2.85984	0.63495
C	-3.28317	-2.99253	-0.52586
H	-4.26447	-3.35294	-0.22746
C	-2.49290	-3.30221	-1.62210
H	-2.71092	-3.99762	-2.42694
C	-1.35375	-2.50637	-1.45644
H	-0.47876	-2.41973	-2.09649
C	-2.39709	-1.92778	3.92374
H	-3.36646	-2.33431	4.20171
C	-1.27375	-1.64819	4.68721
H	-1.13847	-1.80235	5.75347
C	-0.36415	-1.10031	3.77339
H	0.63233	-0.69135	3.93413
C	3.36048	-1.23654	1.28373

H	4.08862	-2.01506	1.55436
H	3.22139	-0.53238	2.11689
H	3.73848	-0.65971	0.43044
C	2.14287	-2.99193	-0.62974
H	2.42182	-2.36896	-1.49020
H	1.26413	-3.59384	-0.90222
H	2.97511	-3.67117	-0.39337
C	1.49835	-3.25798	2.10155
H	0.51366	-3.72617	1.95689
H	1.51712	-2.81689	3.10602
H	2.28320	-4.02584	2.03378
B	-3.13624	-1.35834	1.48768
H	-4.23930	-1.76238	1.78711
H	-1.07035	0.58109	-1.75344
H	4.63392	3.55085	1.29704
H	2.68061	5.07704	1.42458
C	-0.16939	1.72808	-4.01700
C	0.83683	2.27655	-3.02370
C	2.02417	1.29329	-3.08065
C	1.59846	0.21870	-4.06440
H	1.11429	3.29300	-3.33877
O	-1.24880	2.17989	-4.30245
O	2.20380	-0.78346	-4.35987
H	2.94341	1.76490	-3.45852
N	0.34944	0.55821	-4.56238
C	-0.39380	-0.26467	-5.48535
H	0.28114	-1.04213	-5.86340
H	-1.25144	-0.73350	-4.97959
H	-0.77360	0.34826	-6.31348
H	-0.58356	3.01811	-1.53033

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2143.5096698
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.512860
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2145.5175244
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2141.748484
Number of imaginary frequencies: 0

16 + NMN (reactants - exo)

C	-1.02597	-1.39163	-2.47721
C	-1.13309	1.19470	-2.87771
C	-3.25111	-0.11175	-2.18264
O	-0.67418	-2.31043	-3.07144
O	-0.84975	1.91668	-3.72620
O	-4.31798	-0.21969	-2.60298
Cr	-1.56966	0.06627	-1.48433
C	2.47692	-0.25624	-0.37190

C	1.35105	-0.97811	-0.08639
C	0.08299	-0.33281	0.04478
C	0.00390	1.08005	-0.16207
C	1.19710	1.79657	-0.48181
C	2.39970	1.14988	-0.56645
H	-1.06167	-2.14410	0.47718
H	1.40175	-2.05808	0.06911
C	-1.11972	-1.06427	0.34169
C	-1.27999	1.72388	-0.07956
H	1.13202	2.87525	-0.63978
C	-2.41564	1.00584	0.30949
C	-2.33307	-0.39762	0.52714
H	-1.35130	2.79190	-0.28867
H	-3.37870	1.51103	0.38645
H	-3.23125	-0.96324	0.77465
C	2.88857	0.21890	2.89533
C	1.74418	1.19165	2.95724
C	0.61129	0.50455	3.10600
C	0.94231	-0.96099	3.15590
H	1.89341	2.26607	2.86884
O	4.05722	0.44582	2.72742
O	0.18511	-1.89292	3.24223
H	-0.41412	0.86544	3.16704
N	2.32711	-1.04416	3.05802
C	3.07149	-2.27539	2.97693
H	2.37740	-3.10024	3.18075
H	3.50774	-2.40346	1.97457
H	3.88376	-2.28440	3.71626
H	3.44486	-0.75513	-0.44622
H	3.30886	1.71126	-0.78836

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2167.8390907
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.218294
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2169.2313399
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2166.660066
Number of imaginary frequencies: 0

16 + NMN (reactants - endo)

C	-0.49158	-1.39577	-2.74181
C	0.24898	1.11012	-2.90211
C	-2.25317	0.49430	-2.71004
O	-0.31789	-2.35274	-3.35440
O	0.89187	1.74083	-3.61632
O	-3.20306	0.73630	-3.31453
Cr	-0.76142	0.11683	-1.71966
C	2.68390	-1.53676	-0.05890

C	1.35759	-1.86401	0.02754
C	0.35284	-0.84819	0.02412
C	0.75747	0.52103	-0.06356
C	2.15162	0.82298	-0.14467
C	3.08548	-0.17780	-0.14606
H	-1.36005	-2.20562	0.07730
H	1.04178	-2.90675	0.10038
C	-1.05126	-1.16081	0.04390
C	-0.25196	1.54399	-0.12880
H	2.45351	1.87059	-0.20567
C	-1.60600	1.21835	-0.01822
C	-2.00845	-0.14348	0.06848
H	0.05567	2.58490	-0.22857
H	-2.35878	2.00585	-0.05837
H	-3.06863	-0.39614	0.09444
C	0.09793	-1.01032	3.27240
C	1.59797	-0.96121	3.19373
C	1.97750	0.31464	3.11021
C	0.75004	1.18159	3.12863
H	2.20647	-1.86317	3.20101
O	-0.61530	-1.97761	3.33205
O	0.68149	2.38009	3.04577
H	2.97874	0.73309	3.03107
N	-0.33041	0.31313	3.24782
C	-1.70526	0.72955	3.36675
H	-1.83054	1.68378	2.84010
H	-2.34818	-0.03633	2.91539
H	-1.99341	0.86218	4.42084
H	3.44020	-2.32410	-0.06086
H	4.14704	0.06784	-0.21427

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2167.8416794
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.220489
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2169.2335287
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2166.662883
Number of imaginary frequencies: 0

16 + NMN (Transition state - exo)

C	-2.38032	-2.31909	0.39019
C	-1.64495	0.16851	0.16928
C	-4.16401	-0.45138	0.14504
O	-2.12562	-3.30469	-0.14380
O	-0.92429	0.75850	-0.50450
O	-5.05145	-0.25156	-0.55933
Cr	-2.76759	-0.76163	1.29866

C	0.51106	-2.31125	2.79851
C	-0.76200	-2.57940	3.34540
C	-1.82732	-1.61567	3.13291
C	-1.42950	-0.26142	3.01263
C	-0.00458	-0.00120	3.11721
C	0.89760	-0.99547	2.68211
H	-3.51879	-2.99787	3.14473
H	-1.04645	-3.61584	3.54156
C	-3.21594	-1.95128	3.09522
C	-2.42048	0.75599	2.85443
H	0.32173	1.04140	3.12844
C	-3.77998	0.41814	2.85346
C	-4.17965	-0.94174	2.97491
H	-2.11118	1.79300	2.71861
H	-4.53207	1.19362	2.70786
H	-5.23648	-1.20344	2.92176
C	1.47883	-0.42844	5.49586
C	0.00176	-0.49151	5.26409
C	-0.39084	-1.82597	5.38389
C	0.82841	-2.63598	5.69319
H	-0.61761	0.37039	5.50576
O	2.19867	0.53661	5.53098
O	0.91178	-3.81605	5.91942
H	-1.36411	-2.16718	5.73203
N	1.90194	-1.74666	5.65166
C	3.28095	-2.13128	5.82599
H	3.29986	-3.14934	6.23444
H	3.82134	-2.11522	4.86746
H	3.77453	-1.43598	6.51774
H	1.21530	-3.12806	2.63324
H	1.92157	-0.72399	2.42070

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2167.7989467
Gibbs free energy correctio (a.u.) at ωB97X-D/def2-SVP: 0.224068
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2169.1872972
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2166.621342
Number of imaginary frequencies: 1

16 + NMN (Transition state - endo)

C	-0.63049	-1.39486	-3.02693
C	0.10681	1.09440	-3.20466
C	-2.40780	0.47017	-3.32886
O	-0.35196	-2.37698	-3.55626
O	0.85251	1.68956	-3.84651
O	-3.26814	0.67231	-4.06567
Cr	-1.05561	0.15543	-2.12623

C	2.16278	-1.40000	-0.48539
C	0.86244	-1.67091	0.00153
C	-0.18865	-0.70973	-0.26111
C	0.21381	0.64680	-0.35920
C	1.62747	0.90847	-0.18748
C	2.55249	-0.08650	-0.58081
H	-1.87929	-2.09122	-0.30593
H	0.55782	-2.70480	0.18014
C	-1.57503	-1.04578	-0.35351
C	-0.77109	1.66599	-0.54659
H	1.94007	1.95485	-0.15718
C	-2.12740	1.32646	-0.60073
C	-2.53102	-0.03489	-0.50581
H	-0.45728	2.70480	-0.64756
H	-2.87397	2.10320	-0.76617
H	-3.58523	-0.29600	-0.59938
C	-0.17229	-0.98004	2.57984
C	1.23180	-0.95728	2.05677
C	1.62563	0.38025	1.96415
C	0.47742	1.22667	2.41987
H	1.89083	-1.79449	2.27573
O	-0.87005	-1.93158	2.82408
O	0.41844	2.42739	2.50333
H	2.63961	0.75107	2.09607
N	-0.56547	0.34848	2.70810
C	-1.89735	0.75770	3.07769
H	-1.91225	1.85418	3.10603
H	-2.62852	0.39514	2.34086
H	-2.16421	0.35737	4.06567
H	2.87254	-2.21622	-0.63047
H	3.58523	0.18600	-0.80479

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2167.8018975
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.225573
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2169.1891944
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2166.624908
Number of imaginary frequencies: 1

16 + NMN (Product - exo)

C	-1.10789	-1.23550	-2.28743
C	-0.37720	1.22694	-2.51530
C	-2.89010	0.60241	-2.73205
O	-0.79343	-2.23015	-2.77305
O	0.40059	1.79437	-3.14548
O	-3.72173	0.77755	-3.50690
Cr	-1.58881	0.33436	-1.45587

C	1.47434	-1.15355	-0.18360
C	0.34489	-1.38141	0.79793
C	-0.80783	-0.45758	0.44841
C	-0.40956	0.88704	0.32385
C	1.07533	1.08471	0.56986
C	1.85192	0.12107	-0.30136
H	-2.47932	-1.85880	0.39024
H	0.03749	-2.43110	0.87001
C	-2.17642	-0.81266	0.33049
C	-1.37306	1.89930	0.07907
H	1.38793	2.12830	0.44835
C	-2.73044	1.54938	-0.02829
C	-3.13289	0.19109	0.09790
H	-1.05919	2.93538	-0.05418
H	-3.47261	2.31612	-0.25077
H	-4.18173	-0.07748	-0.02854
C	2.73776	0.63106	2.46112
C	1.27478	0.61534	2.04697
C	0.84033	-0.85310	2.18269
C	2.08008	-1.58961	2.66564
H	0.71891	1.28525	2.71882
O	3.48007	1.57767	2.47518
O	2.18363	-2.76982	2.87431
H	0.04554	-0.99270	2.92968
N	3.09927	-0.65901	2.82025
C	4.44029	-1.00578	3.23241
H	4.43576	-2.05898	3.53749
H	5.14581	-0.86373	2.40147
H	4.75307	-0.36790	4.06969
H	1.92159	-1.98278	-0.73246
H	2.64817	0.47040	-0.95929

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2167.8709638
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.230601
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2169.2541557
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2166.68798
Number of imaginary frequencies: 0

16 + NMN (Product - endo)

C	-0.03732	-1.51568	-2.49884
C	0.69023	0.95091	-2.67683
C	-1.78169	0.29864	-3.15178
O	0.33903	-2.51254	-2.93415
O	1.52811	1.51876	-3.22489
O	-2.52759	0.45639	-4.01273

Cr	-0.61829	0.05721	-1.74333
C	2.31334	-1.38685	-0.10188
C	1.07297	-1.61283	0.73560
C	-0.03672	-0.70815	0.23300
C	0.36114	0.63924	0.13625
C	1.80188	0.85718	0.55954
C	2.69029	-0.11026	-0.19255
H	-1.68482	-2.12328	0.04457
H	0.75809	-2.66150	0.78712
C	-1.38469	-1.07649	-0.01016
C	-0.58151	1.64214	-0.20606
H	2.10602	1.90571	0.46179
C	-1.91532	1.27706	-0.45268
C	-2.31754	-0.08413	-0.35433
H	-0.26535	2.68125	-0.30144
H	-2.63774	2.03502	-0.75552
H	-3.34626	-0.36302	-0.58266
C	0.18374	-1.04983	3.06192
C	1.40956	-1.06551	2.16143
C	1.84270	0.40637	2.05677
C	0.83839	1.17496	2.90249
H	2.17578	-1.70510	2.62026
O	-0.49821	-1.98901	3.38062
O	0.79136	2.36663	3.06444
H	2.84928	0.58575	2.45850
N	-0.05838	0.26204	3.44255
C	-1.19660	0.64191	4.24757
H	-1.10092	1.70851	4.48287
H	-2.13065	0.46687	3.69453
H	-1.21936	0.04818	5.17082
H	2.82428	-2.21688	-0.59083
H	3.54959	0.23983	-0.76538

Electronic energy (a.u.) at ωB97xd/def2-SVP: -2167.873368
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.229823
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2169.2559308
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2166.687983
Number of imaginary frequencies: 0

14 + bis(trifluoromethyl)tetrazine (reactants)

Ir	2.10642	-0.03981	-0.07269
C	0.37974	-1.24287	0.34946
H	0.50483	-2.32544	0.44113
C	0.33566	-0.71178	-1.00909
H	0.31452	-1.32613	-1.91026

C	0.38815	0.71041	-1.04799
H	0.41072	1.27401	-1.98191
C	0.47489	1.31107	0.27832
H	0.68063	2.38440	0.30964
C	-0.43303	0.76543	1.32539
C	-0.48367	-0.57389	1.36261
C	3.87952	-1.23572	0.50644
C	4.12223	-0.86145	-0.85420
C	4.17798	0.55366	-0.91389
C	3.96849	1.05863	0.40931
C	3.83349	-0.04957	1.30953
H	4.33526	1.15472	-1.80716
H	4.22923	-1.54604	-1.69315
H	3.80132	-2.25604	0.87794
H	3.73961	-0.00049	2.39157
H	3.97244	2.10938	0.69408
H	-1.01384	1.42405	1.97479
H	-1.11292	-1.15202	2.04233
C	-3.11192	-1.20824	-0.15672
C	-3.18574	1.28648	0.02223
N	-3.79005	0.59772	0.98829
N	-3.74830	-0.69900	0.89614
N	-2.74889	0.78010	-1.12423
N	-2.71189	-0.52009	-1.21856
C	-2.95928	-2.72470	-0.19328
C	-3.12432	2.80136	0.18078
F	-2.56546	-3.17604	0.99213
F	-2.06777	-3.09057	-1.10076
F	-4.12372	-3.29389	-0.49099
F	-4.24152	3.35442	-0.28366
F	-2.99425	3.13171	1.45888
F	-2.09766	3.30041	-0.49162

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-1499.1260436
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.195593
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1500.7401911
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1498.24023
Number of imaginary frequencies: 0

14 + bis(trifluoromethyl)tetrazine (Transition state)

Ir	1.81212	-0.06173	-0.26200
C	0.07709	-1.33014	-0.15922
H	0.21304	-2.41165	-0.09839
C	0.20523	-0.73112	-1.47444
H	0.32052	-1.30434	-2.39492
C	0.22224	0.68982	-1.44847

H	0.35163	1.29336	-2.34744
C	0.10791	1.24327	-0.11218
H	0.26968	2.31827	-0.01194
C	-0.89936	0.64412	0.80063
C	-0.91595	-0.74081	0.77531
C	3.53074	-1.24565	0.47529
C	3.92024	-0.78650	-0.82304
C	3.93723	0.63259	-0.79688
C	3.55828	1.05277	0.51767
C	3.34777	-0.10946	1.33066
H	4.18356	1.28905	-1.62891
H	4.15115	-1.41755	-1.67881
H	3.44000	-2.28773	0.77706
H	3.12613	-0.12643	2.39492
H	3.49235	2.08490	0.85768
H	-1.24633	1.20399	1.66785
H	-1.27659	-1.32351	1.62165
C	-2.97032	-1.23148	-0.11063
C	-2.94105	1.21585	-0.06590
N	-3.71786	0.62151	0.88333
N	-3.73311	-0.65381	0.86002
N	-2.82231	0.65284	-1.29488
N	-2.83762	-0.62694	-1.31827
C	-2.97592	-2.75151	-0.12222
C	-2.91028	2.73500	-0.02194
F	-2.64317	-3.23889	1.07410
F	-2.11418	-3.22827	-1.01559
F	-4.18356	-3.21577	-0.42820
F	-4.10634	3.23889	-0.31019
F	-2.56645	3.17023	1.19123
F	-2.03701	3.22333	-0.89770

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-1500.7211488
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.199907
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1500.7211488
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1498.226893
Number of imaginary frequencies: 1

14 + bis(trifluoromethyl)tetrazine (Product)

Ir	1.87868	-0.02030	-0.14276
C	0.17301	-1.28094	-0.24233
H	0.33641	-2.35931	-0.16857
C	0.42329	-0.69003	-1.53613
H	0.66271	-1.26135	-2.43411
C	0.44074	0.73612	-1.50962
H	0.69447	1.33440	-2.38586

C	0.20439	1.28449	-0.19464
H	0.39408	2.35506	-0.08093
C	-0.94268	0.76544	0.65749
C	-0.96141	-0.76602	0.62903
C	3.50101	-1.21017	0.79690
C	4.02341	-0.75305	-0.45105
C	4.04087	0.67054	-0.42471
C	3.52926	1.09387	0.83952
C	3.21547	-0.06929	1.61856
H	4.38326	1.32350	-1.22493
H	4.35005	-1.38417	-1.27502
H	3.37699	-2.25098	1.09064
H	2.87462	-0.08421	2.65106
H	3.43067	2.12583	1.17161
H	-0.81499	1.13191	1.68425
H	-0.84319	-1.17339	1.64140
C	-2.39740	-1.17843	0.16883
C	-2.36794	1.22967	0.21359
N	-3.29837	0.63334	1.18763
N	-3.31341	-0.59613	1.16477
N	-2.63969	0.66941	-1.11006
N	-2.65476	-0.56290	-1.13297
C	-2.65323	-2.68158	0.08377
C	-2.58689	2.74074	0.18456
F	-2.29055	-3.27769	1.22116
F	-1.95464	-3.23269	-0.90726
F	-3.93745	-2.93474	-0.12887
F	-3.86444	3.03295	-0.01795
F	-2.21026	3.28513	1.34315
F	-1.87459	3.31105	-0.78563

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-1499.1815294
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.203996
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -1500.7898469
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -1498.29743
Number of imaginary frequencies: 0

14 + Cyclopentadiene (reactants - exo)

Ir	1.02740	0.03170	-0.07531
C	-0.91976	-0.73118	0.40283
H	-1.01100	-1.78504	0.68148
C	-0.79489	-0.45536	-1.02344
H	-0.87956	-1.20952	-1.80839
C	-0.46031	0.90390	-1.29524
H	-0.26604	1.27295	-2.30429
C	-0.31897	1.70108	-0.08078

H	0.10402	2.70213	-0.20877
C	-1.36838	1.52971	0.96398
C	-1.68293	0.25562	1.21679
C	2.49963	-1.36370	0.82546
C	2.89981	-1.26258	-0.54534
C	3.23200	0.09050	-0.80383
C	3.04046	0.83059	0.40694
C	2.63496	-0.07584	1.44093
H	3.56040	0.50204	-1.75609
H	2.92465	-2.08003	-1.26309
H	2.20256	-2.27997	1.33273
H	2.48288	0.16185	2.49090
H	3.23238	1.89436	0.53622
H	-1.87895	2.39028	1.40142
H	-2.49188	-0.06293	1.87665
C	-4.24897	-1.08619	-0.71847
C	-4.36040	0.38946	-0.95234
C	-5.13560	0.86937	0.23695
C	-5.41966	-0.17943	1.03548
C	-4.86549	-1.40092	0.43878
H	-5.40774	1.91082	0.40980
H	-5.96874	-0.14152	1.97753
H	-3.73720	-1.77509	-1.39064
H	-4.94568	-2.39772	0.87513
H	-4.86705	0.62494	-1.90578
H	-3.36393	0.86529	-1.00010

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-723.6418022
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.234013
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –724.3260204
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -722.7949832
Number of imaginary frequencies: 0

14 + Cyclopentadiene (reactants - endo)

Ir	0.98141	-0.07821	0.05344
C	-0.69687	-1.36828	0.41708
H	-0.50777	-2.43947	0.53508
C	-0.70499	-0.86460	-0.94976
H	-0.63434	-1.49280	-1.83981
C	-0.72887	0.55769	-1.01226
H	-0.67791	1.10688	-1.95446
C	-0.73850	1.18082	0.30457
H	-0.58634	2.26407	0.32572
C	-1.66217	0.60276	1.32011
C	-1.64209	-0.73223	1.37752
C	2.79597	-1.16096	0.73699

C	3.09259	-0.78176	-0.61150
C	3.06359	0.63346	-0.68245
C	2.75086	1.13383	0.62190
C	2.63476	0.02630	1.52445
H	3.23366	1.23696	-1.57176
H	3.28771	-1.46399	-1.43642
H	2.76164	-2.18139	1.11483
H	2.47778	0.07696	2.59907
H	2.67651	2.18481	0.89593
H	-2.33986	1.23984	1.89163
H	-2.30006	-1.33701	2.00518
C	-4.68173	1.32424	-0.18090
C	-5.07578	0.01251	0.42918
C	-4.56740	-0.99346	-0.55928
H	-4.66852	-2.07252	-0.44191
H	-3.51731	-0.81327	-2.45774
H	-4.88709	2.29567	0.26953
H	-3.64688	1.85750	-2.02056
H	-6.16912	-0.06446	0.57291
H	-4.62028	-0.12868	1.42514
C	-3.98136	-0.34823	-1.58708
C	-4.05076	1.09748	-1.35025

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-723.6414312
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.232666
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -724.3253272
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -722.7945917
Number of imaginary frequencies: 0

14 + Cyclopentadiene (Transition state - exo)

Ir	0.90102	-0.01339	-0.16316
C	-0.86594	-1.26380	-0.13087
H	-0.72295	-2.34588	-0.05302
C	-0.63875	-0.68810	-1.43776
H	-0.44568	-1.26919	-2.34173
C	-0.61173	0.74172	-1.42488
H	-0.39666	1.33137	-2.31826
C	-0.81764	1.30171	-0.10771
H	-0.63399	2.37603	-0.01019
C	-1.85042	0.72516	0.80627
C	-1.87644	-0.66540	0.79388
C	2.56403	-1.20038	0.71614
C	3.08673	-0.75751	-0.54242
C	3.11250	0.65697	-0.52914
C	2.60599	1.09508	0.73767
C	2.32234	-0.05546	1.54373

H	3.43751	1.30308	-1.34214
H	3.38827	-1.39977	-1.36743
H	2.44494	-2.23875	1.02101
H	2.00823	-0.05954	2.58463
H	2.52464	2.13130	1.06167
H	-2.09535	1.29427	1.69969
H	-2.14259	-1.24078	1.67715
C	-3.95802	-1.07663	-0.06971
C	-3.80729	0.08208	-1.00821
C	-3.91483	1.22937	-0.04992
C	-4.68445	0.78371	1.02607
C	-4.71078	-0.62100	1.01399
H	-3.81041	2.27397	-0.34955
H	-5.08324	1.41503	1.82165
H	-3.89294	-2.11909	-0.38741
H	-5.13328	-1.25050	1.79869
H	-4.70216	0.10444	-1.66269
H	-2.92976	0.07125	-1.66015

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-723.601218
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.240555
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -724.2805582
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -722.7538649
Number of imaginary frequencies: 1

14 + Cyclopentadiene (Transition state - endo)

Ir	0.88960	-0.00941	-0.08577
C	-0.86402	-1.26474	-0.08288
H	-0.71896	-2.34803	-0.02886
C	-0.65012	-0.65757	-1.37781
H	-0.45890	-1.21472	-2.29704
C	-0.62858	0.76839	-1.33108
H	-0.41961	1.37847	-2.21204
C	-0.82535	1.29567	0.00099
H	-0.64768	2.36821	0.12567
C	-1.87789	0.69575	0.87330
C	-1.89882	-0.69172	0.82789
C	2.55934	-1.21227	0.75947
C	3.06356	-0.73752	-0.49407
C	3.08516	0.67814	-0.44701
C	2.59432	1.08373	0.83583
C	2.31860	-0.08750	1.61479
H	3.40273	1.34426	-1.24667
H	3.36154	-1.35840	-1.33653
H	2.44627	-2.25797	1.04057
H	2.01287	-0.11751	2.65776

H	2.51272	2.11140	1.18583
H	-2.18394	1.24824	1.76133
H	-2.22207	-1.29160	1.67828
C	-3.91150	1.21485	-0.00089
C	-4.49394	0.04454	0.74423
C	-3.94588	-1.09153	-0.07610
H	-4.12179	-2.14231	0.16189
H	-3.49777	-1.20791	-2.23620
H	-4.05616	2.25267	0.30525
H	-3.45793	1.45826	-2.14924
H	-5.59498	0.06506	0.61797
H	-4.28610	0.00631	1.82158
C	-3.73609	-0.60261	-1.36111
C	-3.71506	0.80461	-1.31521

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-723.606972
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.240525
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -724.2859888
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -722.7599371
Number of imaginary frequencies: 1

14 + Cyclopentadiene (Product - exo)

Ir	0.87374	-0.01636	-0.15376
C	-0.85884	-1.26685	-0.27317
H	-0.69623	-2.34829	-0.19520
C	-0.55392	-0.69086	-1.56017
H	-0.27872	-1.26926	-2.44461
C	-0.52579	0.74006	-1.54676
H	-0.22767	1.32364	-2.42031
C	-0.80832	1.30341	-0.24912
H	-0.60329	2.37597	-0.15099
C	-1.95991	0.80707	0.60998
C	-1.99038	-0.74176	0.59546
C	2.45399	-1.20906	0.85943
C	3.04170	-0.76688	-0.36624
C	3.06891	0.65468	-0.35126
C	2.49827	1.09315	0.88379
C	2.14578	-0.05989	1.66031
H	3.45296	1.29842	-1.14000
H	3.40105	-1.40809	-1.16857
H	2.31051	-2.24632	1.15680
H	1.75757	-0.06315	2.67596
H	2.39454	2.12868	1.20296
H	-1.79966	1.19195	1.62764
H	-1.84582	-1.15165	1.60567
C	-3.44364	-1.05591	0.10514

C	-3.68402	0.08045	-0.90559
C	-3.39952	1.18729	0.12623
C	-4.32855	0.74221	1.24685
C	-4.35487	-0.59577	1.23426
H	-3.50337	2.22860	-0.20753
H	-4.78825	1.40502	1.98182
H	-3.58824	-2.08588	-0.24808
H	-4.84055	-1.25369	1.95682
H	-4.71990	0.10428	-1.27360
H	-2.99666	0.07498	-1.76092

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-723.6924242
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.247447
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -724.3678392
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -722.838857
Number of imaginary frequencies: 0

14 + Cyclopentadiene (Product - endo)

Ir	0.84884	-0.01206	-0.05475
C	-0.87964	-1.27106	-0.21094
H	-0.70965	-2.35297	-0.16019
C	-0.57720	-0.65695	-1.47970
H	-0.29912	-1.20967	-2.37951
C	-0.55437	0.77157	-1.43202
H	-0.25782	1.37388	-2.29328
C	-0.83840	1.30908	-0.12483
H	-0.63401	2.37923	-0.00224
C	-1.98772	0.78199	0.71310
C	-2.01244	-0.76457	0.66148
C	2.43179	-1.22213	0.92932
C	3.01415	-0.75015	-0.28831
C	3.03681	0.67062	-0.24079
C	2.46849	1.07851	1.00627
C	2.12424	-0.09304	1.75822
H	3.41707	1.33372	-1.01519
H	3.37392	-1.37180	-1.10569
H	2.29287	-2.26651	1.20307
H	1.73953	-0.12091	2.77483
H	2.36262	2.10617	1.34934
H	-1.82845	1.12395	1.74734
H	-1.86525	-1.17961	1.67046
C	-3.45031	1.16952	0.29863
C	-4.22144	0.03374	1.00134
C	-3.48621	-1.07672	0.22368
H	-3.79864	-2.11262	0.41162
H	-3.68894	-1.19701	-2.08750

H	-3.72971	2.20003	0.55552
H	-3.64663	1.44998	-1.99918
H	-5.30321	0.05764	0.80308
H	-4.04603	-0.00535	2.08857
C	-3.66883	-0.57147	-1.19406
C	-3.64745	0.76595	-1.14943

Electronic energy (a.u.) at ωB97X-D/def2-SVP:-723.692282
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.247757
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -724.3667088
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -722.8378096
Number of imaginary frequencies: 0

11 + Cyclopentadiene (Reactants - endo)

Fe	1.51066	0.03932	0.13298
C	2.67973	-1.21656	-0.39117
C	1.74477	0.02226	1.91089
C	2.60865	1.37088	-0.35696
C	0.00221	-0.69093	-1.04155
C	-0.03645	0.71648	-1.02291
C	-0.20974	1.29181	0.28192
C	-1.16746	0.62132	1.19362
C	-1.13069	-0.71668	1.17590
C	-0.13825	-1.30921	0.24749
H	0.20424	-1.24975	-1.95736
H	0.13394	1.30958	-1.92347
H	-0.10298	2.37620	0.36697
H	-1.86568	1.20873	1.79215
H	-1.79516	-1.35716	1.75820
H	0.02794	-2.38797	0.30391
O	1.87299	0.01082	3.04473
O	3.38170	-2.06105	-0.70713
O	3.26298	2.26068	-0.64999
C	-4.02730	1.07537	-0.65072
C	-4.50745	-0.12515	0.10825
C	-3.96197	-1.27477	-0.68462
C	-3.28832	-0.79804	-1.75052
C	-3.32905	0.66770	-1.72937
H	-4.10976	-2.32312	-0.42445
H	-2.78588	-1.39501	-2.51287
H	-4.23290	2.10595	-0.36057
H	-2.86115	1.31339	-2.47379
H	-5.61096	-0.15668	0.16779
H	-4.14271	-0.13004	1.15033

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2029.1206179
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.173701
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2030.1451964
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2028.08410
Number of imaginary frequencies: 0

11 + Cyclopentadiene (Reactants - exo)

Fe	1.60238	0.03890	0.01365
C	3.00639	-0.86520	-0.64432
C	1.80079	-0.23383	1.77553
C	2.42958	1.61801	-0.19468
C	0.28844	-0.75171	-1.34034
C	-0.02616	0.59931	-1.09193
C	-0.33110	0.89950	0.28022
C	-1.15764	-0.08551	1.01802
C	-0.86044	-1.36952	0.78338
C	0.24786	-1.59688	-0.17674
H	0.61436	-1.09623	-2.32379
H	0.04111	1.35947	-1.87275
H	-0.44465	1.95344	0.54535
H	-1.98342	0.24617	1.64888
H	-1.40702	-2.21079	1.21316
H	0.62322	-2.61742	-0.28839
O	1.90717	-0.41271	2.89717
O	3.86647	-1.49510	-1.05504
O	2.90338	2.65173	-0.30458
C	-4.52788	-0.58376	-0.18969
C	-3.67352	-0.15487	-1.34409
C	-3.51772	1.31981	-1.12834
C	-4.18380	1.67861	-0.01204
C	-4.81535	0.48982	0.57388
H	-2.94894	1.97801	-1.78551
H	-4.25250	2.68621	0.40079
H	-4.84953	-1.61074	-0.01544
H	-5.41729	0.49048	1.48379
H	-4.14195	-0.38601	-2.31797
H	-2.69648	-0.67171	-1.33599

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2029.1206202
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.172961
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2030.1454897
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2028.08391
Number of imaginary frequencies: 0

11 + Cyclopentadiene (Transition state - endo)

Fe	1.43600	0.00803	-0.03540
C	2.66368	-1.24817	-0.38304
C	1.38574	-0.01726	1.75599
C	2.59296	1.33834	-0.34864
C	0.12698	-0.71471	-1.43414
C	0.08794	0.69596	-1.41524
C	-0.29944	1.26997	-0.16679
C	-1.37622	0.61931	0.61831
C	-1.33833	-0.77320	0.59918
C	-0.22784	-1.34259	-0.20200
H	0.48109	-1.26539	-2.30759
H	0.41090	1.28854	-2.27320
H	-0.19738	2.35348	-0.06281
H	-1.76815	1.15850	1.48066
H	-1.70024	-1.35634	1.44591
H	-0.06666	-2.42132	-0.12723
O	1.33477	-0.03389	2.89767
O	3.40763	-2.09158	-0.59135
O	3.28944	2.22648	-0.53380
C	-3.34989	1.03792	-0.42117
C	-3.94194	-0.14290	0.29829
C	-3.28744	-1.26902	-0.45421
C	-2.99133	-0.79233	-1.72726
C	-3.02951	0.61471	-1.70714
H	-3.44020	-2.32202	-0.21050
H	-2.66184	-1.40192	-2.56928
H	-3.55939	2.07369	-0.14761
H	-2.73423	1.26508	-2.53114
H	-5.02895	-0.16926	0.08497
H	-3.82108	-0.15522	1.38937

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2029.0877115
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.180602
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2030.107906
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2028.05152
Number of imaginary frequencies: 1

11 + Cyclopentadiene (Transition state - exo)

Fe	1.41383	-0.01879	-0.02797
C	2.53650	-1.37534	-0.35278
C	1.35314	-0.01599	1.76631
C	2.68672	1.19819	-0.35173

C	0.05187	-0.64708	-1.42201
C	0.13429	0.76487	-1.42140
C	-0.22720	1.39054	-0.19240
C	-1.33671	0.84095	0.62443
C	-1.41809	-0.55324	0.62385
C	-0.38003	-1.22749	-0.19351
H	0.37076	-1.23846	-2.28233
H	0.51986	1.31586	-2.28123
H	-0.03125	2.46237	-0.10287
H	-1.62972	1.41441	1.50095
H	-1.77584	-1.08945	1.49991
H	-0.31010	-2.31492	-0.10491
O	1.30807	-0.01382	2.90804
O	3.20585	-2.28222	-0.54643
O	3.45705	2.02119	-0.54468
C	-3.42413	-0.89138	-0.41417
C	-3.14282	0.24768	-1.34632
C	-3.28971	1.41102	-0.41329
C	-4.16473	1.01001	0.59805
C	-4.24658	-0.39204	0.59752
H	-3.11951	2.44696	-0.71265
H	-4.60557	1.66747	1.34877
H	-3.37562	-1.93985	-0.71433
H	-4.76096	-0.99431	1.34775
H	-3.97129	0.29633	-2.08111
H	-2.21056	0.19347	-1.91654

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2029.0823695
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.180613
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2030.103064
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2028.04590
Number of imaginary frequencies: 1

11 + Cyclopentadiene (Product - endo)

Fe	1.22130	0.03210	0.08185
C	2.46641	-1.23888	-0.13889
C	1.01071	0.00208	1.84808
C	2.39535	1.37442	-0.10302
C	0.06682	-0.68570	-1.44062
C	0.02832	0.72783	-1.42105
C	-0.43752	1.30194	-0.20031
C	-1.63570	0.72407	0.52255
C	-1.59347	-0.82625	0.50111
C	-0.36617	-1.31784	-0.23657
H	0.50025	-1.23109	-2.28168

H	0.43078	1.31907	-2.24637
H	-0.30741	2.38430	-0.09271
H	-1.61803	1.08880	1.56096
H	-1.55519	-1.21804	1.52905
H	-0.17727	-2.39408	-0.15885
O	0.83434	-0.01825	2.97788
O	3.22847	-2.07911	-0.27563
O	3.11051	2.25826	-0.21620
C	-3.05966	1.04135	-0.05949
C	-3.85553	-0.11308	0.58128
C	-2.99849	-1.20436	-0.09055
C	-3.04599	-0.73128	-1.52964
C	-3.08245	0.60634	-1.51114
H	-3.28608	-2.24919	0.08564
H	-2.95000	-1.37274	-2.40669
H	-3.40356	2.06372	0.14528
H	-3.02220	1.27606	-2.37006
H	-4.90887	-0.13743	0.26694
H	-3.79807	-0.12673	1.68144

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2029.1696805
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.188374
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2030.1844256
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: -2028.12709
Number of imaginary frequencies: 0

11 + Cyclopentadiene (Product - exo)

Fe	1.26782	-0.07409	-0.03951
C	2.40195	-1.44997	-0.23173
C	1.04548	-0.06193	1.72596
C	2.55443	1.16057	-0.23050
C	0.06480	-0.71206	-1.55918
C	0.14734	0.70099	-1.55853
C	-0.27627	1.32385	-0.34560
C	-1.52436	0.86649	0.38570
C	-1.61490	-0.68357	0.38498
C	-0.42851	-1.28246	-0.34680
H	0.45473	-1.30701	-2.38788
H	0.60393	1.24726	-2.38671
H	-0.05865	2.39328	-0.25101
H	-1.47968	1.26051	1.41132
H	-1.61647	-1.08106	1.41023
H	-0.33690	-2.37005	-0.25320
O	0.86542	-0.05194	2.85482
O	3.09038	-2.35376	-0.35062

O	3.34340	1.97819	-0.34858
C	-3.01551	-0.94693	-0.26847
C	-3.09286	0.18122	-1.31257
C	-2.88473	1.29174	-0.26743
C	-3.95016	0.90055	0.74587
C	-4.02820	-0.43529	0.74525
H	-2.90727	2.33126	-0.62085
H	-4.46224	1.59239	1.41637
H	-3.15890	-1.97643	-0.62285
H	-4.61738	-1.06342	1.41514
H	-4.07782	0.23898	-1.79717
H	-2.31387	0.13608	-2.08438

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2029.1695234
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.188225
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2030.1851623
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2028.12794
Number of imaginary frequencies: 0

11 + bis(trifluoromethyl)tetrazine (Reactants)

C	-2.54903	-1.10008	-0.45589
C	-2.40697	1.39864	-0.40265
N	-3.17933	0.82036	0.51552
N	-3.25314	-0.47754	0.48785
N	-1.88071	0.79079	-1.45815
N	-1.95474	-0.51149	-1.48589
C	-2.54043	-2.62433	-0.41434
C	-2.22585	2.90894	-0.29629
F	-2.44396	-3.05097	0.83877
F	-1.51762	-3.10707	-1.10409
F	-3.66572	-3.10218	-0.93533
F	-3.28923	3.53291	-0.79219
F	-2.08304	3.26796	0.97349
F	-1.15421	3.30188	-0.96870
Fe	2.68461	-0.15582	0.19490
C	3.74385	-1.50009	-0.35515
C	2.94780	-0.20960	1.97030
C	3.88935	1.08385	-0.29845
C	1.11465	-0.74664	-0.97564
C	1.19377	0.65801	-0.94484
C	1.08306	1.23569	0.36863
C	0.07944	0.63994	1.28224
C	0.00392	-0.70097	1.25283
C	0.93659	-1.36508	0.31160

H	1.24329	-1.31234	-1.89971
H	1.38733	1.24553	-1.84363
H	1.27367	2.30748	0.46023
H	-0.53808	1.27250	1.92279
H	-0.68226	-1.28759	1.86668
H	1.00550	-2.45447	0.35581
O	3.09064	-0.24246	3.10106
O	4.37185	-2.39324	-0.68749
O	4.61441	1.91457	-0.59298

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2804.6034195
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.135962
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2806.5581202
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2803.52767
Number of imaginary frequencies: 0

11 + bis(trifluoromethyl)tetrazine (Transition state)

C	-2.74514	-1.23686	-0.74535
C	-2.60681	1.20681	-0.69289
N	-3.50917	0.65161	0.16645
N	-3.58119	-0.62070	0.13913
N	-2.38363	0.63478	-1.90436
N	-2.45592	-0.64235	-1.93178
C	-2.82791	-2.75553	-0.76303
C	-2.51771	2.72448	-0.64537
F	-2.63642	-3.25624	0.45808
F	-1.90755	-3.27516	-1.57055
F	-4.02112	-3.15643	-1.18642
F	-3.65705	3.27516	-1.04835
F	-2.27395	3.14768	0.59557
F	-1.54265	3.17105	-1.43213
Fe	1.98604	-0.28755	-0.32504
C	3.10841	-1.64291	-0.71189
C	2.02227	-0.32809	1.47173
C	3.25514	0.94775	-0.65640
C	0.60416	-0.88331	-1.71778
C	0.68361	0.51920	-1.68778
C	0.39882	1.11395	-0.41322
C	-0.71725	0.54741	0.37282
C	-0.79591	-0.84101	0.34310
C	0.25098	-1.49590	-0.46905
H	0.85365	-1.45716	-2.61126
H	0.99842	1.09878	-2.55660
H	0.57973	2.18444	-0.30485
H	-1.11615	1.11069	1.21568

H	-1.25792	-1.39108	1.16212
H	0.30963	-2.58360	-0.40684
O	2.02283	-0.35254	2.61126
O	3.77740	-2.53517	-0.94618
O	4.02112	1.76799	-0.85400

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2804.5864888
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.138873
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2806.5367142
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2803.51268
Number of imaginary frequencies: 1

11 + bis(trifluoromethyl)tetrazine (Product)

C	-1.87509	-1.09881	-0.07626
C	-1.73888	1.30567	-0.02471
N	-2.80092	0.75675	0.83412
N	-2.87044	-0.47070	0.80782
N	-1.87697	0.75315	-1.37139
N	-1.94667	-0.47721	-1.39777
C	-2.19007	-2.58955	-0.19271
C	-1.88330	2.82604	-0.07661
F	-1.98702	-3.19665	0.97722
F	-1.40778	-3.17430	-1.09874
F	-3.45079	-2.78097	-0.55200
F	-3.11346	3.17374	-0.42440
F	-1.61589	3.35581	1.11770
F	-1.03776	3.35692	-0.95869
Fe	2.37455	-0.13729	0.13011
C	3.51613	-1.51189	-0.10862
C	2.20413	-0.16566	1.90304
C	3.66455	1.10862	-0.05241
C	1.15823	-0.74140	-1.40208
C	1.23789	0.66514	-1.37193
C	0.85781	1.25456	-0.12323
C	-0.39658	0.77886	0.58558
C	-0.48338	-0.75343	0.55273
C	0.71102	-1.33695	-0.17879
H	1.51067	-1.32155	-2.25662
H	1.65563	1.23778	-2.20175
H	1.06587	2.31999	-0.00005
H	-0.38691	1.14242	1.62163
H	-0.51730	-1.15969	1.57228
H	0.79721	-2.42334	-0.10174
O	2.03178	-0.18009	3.03132
O	4.20635	-2.40624	-0.25608

O	4.45165	1.92485	-0.16318

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2804.6531309
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.145469
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2806.6008712
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2803.57973
Number of imaginary frequencies: 0

11 + Danishefsky diene (Reactants - endo)

Fe	2.18785	-0.20557	0.18920
C	3.61806	-0.97916	-0.56835
C	2.91014	0.50785	1.66691
C	2.22551	1.17438	-0.94901
C	0.97768	-1.83186	-0.09325
C	0.24351	-0.64530	-0.27989
C	0.21093	0.22125	0.86484
C	0.04485	-0.41784	2.19085
C	0.74078	-1.54790	2.37044
C	1.56514	-1.97142	1.21211
H	1.14549	-2.54079	-0.90632
H	-0.20834	-0.37203	-1.23435
H	-0.23165	1.20851	0.72312
H	-0.63772	0.01063	2.92709
H	0.69747	-2.15833	3.27421
H	2.25996	-2.80198	1.36129
O	3.35455	0.95819	2.61677
O	4.52355	-1.51767	-1.01130
O	2.17577	2.07854	-1.64921
C	-2.91719	0.39716	-0.24870
H	-3.92257	0.44574	1.60843
C	-3.38515	1.01495	0.85070
H	-3.25563	2.08565	1.01561
C	-2.98444	-1.05664	-0.47285
H	-3.15217	-1.37019	-1.50569
C	-2.75636	-1.94432	0.50966
O	-2.76919	-3.27884	0.42295
O	-2.30663	1.03015	-1.27910
C	-3.06004	-3.85537	-0.82243
H	-3.04019	-4.94304	-0.68486
H	-2.30881	-3.57123	-1.58009
H	-4.05775	-3.55037	-1.18334
H	-2.49470	-1.62052	1.52074
Si	-2.21023	2.67358	-1.70188
C	-1.37434	2.64532	-3.37042
H	-1.94022	2.03253	-4.08839

H	-1.28925	3.66389	-3.78112
H	-0.35748	2.23170	-3.28745
C	-3.94052	3.37926	-1.80533
H	-4.45594	3.34740	-0.83415
H	-3.90855	4.42825	-2.14071
H	-4.54632	2.80991	-2.52724
C	-1.14969	3.61505	-0.47572
H	-0.11440	3.24129	-0.48974
H	-1.11753	4.68042	-0.75638
H	-1.52533	3.55267	0.55625

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2589.1035241
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.292670
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2590.5471627
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2587.59577
Number of imaginary frequencies: 0

11 + Danishefsky diene (Reactants - exo)

Fe	2.02312	0.09892	-0.25814
C	1.75296	-0.87976	-1.73844
C	2.11468	-1.17963	0.98928
C	3.75803	0.35692	-0.64458
C	0.52846	1.42153	-0.71548
C	1.61018	2.10018	-0.12054
C	1.94252	1.64838	1.20416
C	0.81100	1.33987	2.11370
C	-0.21590	0.69374	1.54676
C	-0.04641	0.39007	0.10484
H	0.21313	1.61999	-1.74142
H	2.19117	2.84782	-0.66414
H	2.86043	2.04078	1.64952
H	0.83283	1.66277	3.15594
H	-1.14238	0.41685	2.05169
H	-0.79020	-0.25836	-0.36008
O	2.14510	-1.98666	1.79693
O	1.51330	-1.51088	-2.65989
O	4.86754	0.55212	-0.83425
C	-3.59655	-0.49013	0.08431
H	-4.81587	-0.59802	-1.63633
C	-4.32239	-1.14820	-0.83547
H	-4.46057	-2.22961	-0.79898
C	-3.31356	0.95665	0.04890
H	-3.24274	1.44957	1.02051
C	-2.99770	1.59731	-1.08697
O	-2.61082	2.87151	-1.22751

O	-3.00677	-1.07488	1.15522
C	-2.49340	3.65297	-0.06476
H	-2.14571	4.64365	-0.38067
H	-1.76430	3.21672	0.64120
H	-3.46623	3.75506	0.44673
H	-2.99729	1.07982	-2.05075
Si	-2.46924	-2.66770	1.41206
C	-1.47964	-2.56017	2.99042
H	-2.08940	-2.15242	3.81142
H	-1.12539	-3.55853	3.29250
H	-0.59762	-1.91491	2.86106
C	-3.93163	-3.81873	1.63329
H	-4.49222	-3.97936	0.70053
H	-3.58519	-4.80252	1.98921
H	-4.63004	-3.41530	2.38294
C	-1.39406	-3.18254	-0.03242
H	-0.46384	-2.59411	-0.05028
H	-1.11785	-4.24561	0.05197
H	-1.90885	-3.04053	-0.99487

Electronic energy (a.u.) at ωB97X-D/def2-SVP: -2589.1040075
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.293116
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2590.5478186
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2587.59576
Number of imaginary frequencies: 0

11 + Danishefsky diene (Transition state - endo)

Fe	1.64922	0.00026	0.20078
C	2.81521	-1.21497	-0.40667
C	1.89024	-0.11614	1.97032
C	2.71328	1.36962	-0.23315
C	0.12466	-0.71704	-0.97618
C	0.08726	0.69260	-0.91485
C	-0.07868	1.22333	0.40310
C	-1.04001	0.54616	1.32278
C	-0.98389	-0.84735	1.26563
C	-0.02659	-1.38065	0.27700
H	0.34111	-1.24090	-1.90950
H	0.24459	1.30887	-1.80117
H	0.02609	2.30566	0.51800
H	-1.24426	1.03819	2.27507
H	-1.22272	-1.45942	2.13526
H	0.16444	-2.45704	0.30180
O	2.02319	-0.18105	3.10403
O	3.52017	-2.03593	-0.77888

O	3.35175	2.28421	-0.48921
C	-3.02511	0.65546	-0.65310
H	-3.46676	0.80966	1.43257
C	-2.93105	1.25886	0.59659
H	-2.81714	2.34283	0.66403
C	-3.09157	-0.74742	-0.78143
H	-2.95943	-1.14454	-1.78838
C	-3.04965	-1.57661	0.32242
O	-2.97926	-2.91833	0.28386
O	-2.79322	1.33337	-1.80140
C	-2.67730	-3.54108	-0.93725
H	-2.55835	-4.61090	-0.72666
H	-1.74147	-3.15126	-1.37154
H	-3.49172	-3.40871	-1.67049
H	-3.41018	-1.24732	1.29518
Si	-3.02380	2.96135	-2.20542
C	-2.89106	2.97853	-4.06770
H	-3.66507	2.34183	-4.52252
H	-3.01148	3.99995	-4.46188
H	-1.90871	2.60252	-4.39280
C	-4.71835	3.51057	-1.62941
H	-4.81446	3.46165	-0.53442
H	-4.91447	4.54894	-1.94124
H	-5.50090	2.87054	-2.06562
C	-1.67495	4.03165	-1.46032
H	-0.67640	3.65565	-1.73200
H	-1.76010	5.06052	-1.84639
H	-1.73013	4.08331	-0.36274

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2589.064556
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.299676
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: -2590.5041456
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2587.55571
Number of imaginary frequencies: 1

11 + Danishefsky diene (Transition state - exo)

Fe	1.42644	0.06479	-0.34167
C	2.37130	-1.17036	-1.22673
C	2.01421	-0.14796	1.33629
C	2.47332	1.39700	-0.92581
C	-0.33688	-0.44077	-1.23428
C	-0.29737	0.95812	-1.03136
C	-0.17619	1.36908	0.33051
C	-0.91573	0.63482	1.37579
C	-1.00287	-0.74338	1.16701
C	-0.24788	-1.21471	-0.03278

H	-0.35579	-0.87571	-2.23540
H	-0.25659	1.65659	-1.86954
H	0.02026	2.42849	0.51331
H	-0.95425	1.05799	2.37832
H	-1.04518	-1.41909	2.02233
H	-0.13827	-2.29708	-0.14641
O	2.37106	-0.29498	2.41221
O	2.94056	-2.00292	-1.76673
O	3.10696	2.28716	-1.26412
C	-3.78876	-0.72065	1.59385
H	-2.88763	-0.71124	-0.34210
C	-3.00162	-1.26853	0.58707
H	-2.94890	-2.35234	0.46486
C	-3.83225	0.67357	1.79958
H	-4.30295	1.01231	2.72358
C	-3.08476	1.53640	1.02036
O	-2.95564	2.85683	1.22684
O	-4.33903	-1.46570	2.57985
C	-3.29787	3.37068	2.48683
H	-2.98891	4.42298	2.49698
H	-2.77660	2.82949	3.29594
H	-4.38504	3.31526	2.66759
H	-2.81241	1.28947	-0.00530
Si	-4.46156	-3.13936	2.80133
C	-5.43607	-3.30796	4.38440
H	-6.42633	-2.83738	4.28711
H	-5.58521	-4.36847	4.64211
H	-4.91069	-2.82382	5.22176
C	-5.38402	-3.91367	1.36598
H	-4.83889	-3.82008	0.41516
H	-5.55189	-4.98631	1.55463
H	-6.36727	-3.43447	1.23919
C	-2.75035	-3.88097	3.00464
H	-2.19449	-3.35291	3.79535
H	-2.82573	-4.94061	3.29784
H	-2.15402	-3.83221	2.08114

Electronic energy (a.u.) at ωB97X-D/def2-SVP: -2589.060056
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.297598
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2590.5007058
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2587.55144
Number of imaginary frequencies: 1

11 + Danishefsky diene (Product - endo)

Fe	2.10983	-0.49019	0.94343

C	3.34297	-1.75549	0.62724
C	1.89007	-0.66219	2.69733
C	3.29281	0.85625	0.87256
C	0.94824	-1.08265	-0.63110
C	0.92384	0.32399	-0.50499
C	0.47727	0.78466	0.77346
C	-0.76888	0.18560	1.41062
C	-0.73226	-1.35640	1.28177
C	0.52129	-1.78447	0.53775
H	1.37111	-1.57223	-1.51126
H	1.32098	0.98103	-1.28134
H	0.61011	1.85377	0.97594
H	-0.75456	0.45355	2.47759
H	-0.68710	-1.80720	2.28439
H	0.69847	-2.86352	0.55455
O	1.69700	-0.76859	3.81934
O	4.09563	-2.59091	0.42712
O	4.01266	1.74261	0.83476
C	-2.41876	0.19956	-0.50991
H	-2.88298	0.69269	1.51215
C	-2.04176	0.82542	0.80808
H	-1.88930	1.90989	0.71579
C	-2.40649	-1.13632	-0.60000
H	-2.72318	-1.61750	-1.52487
C	-2.02017	-1.92851	0.62057
O	-1.89697	-3.32338	0.44411
O	-2.81233	0.96614	-1.54560
C	-1.62890	-3.84056	-0.82557
H	-1.30373	-4.88101	-0.68280
H	-0.82617	-3.29812	-1.35564
H	-2.52266	-3.85219	-1.47649
H	-2.82265	-1.81853	1.37619
Si	-2.72885	2.61024	-1.91829
C	-3.40387	2.71026	-3.65530
H	-4.43828	2.33612	-3.69495
H	-3.40211	3.75020	-4.01840
H	-2.79806	2.10483	-4.34658
C	-3.80228	3.60369	-0.74472
H	-3.41497	3.61415	0.28507
H	-3.86834	4.64925	-1.08683
H	-4.82396	3.19359	-0.71817
C	-0.94615	3.18970	-1.86750
H	-0.32836	2.58706	-2.55135
H	-0.87580	4.24203	-2.18673
H	-0.50987	3.11360	-0.86025

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2589.1591695
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.305592
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2590.5936142
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2587.64376
Number of imaginary frequencies: 0

11 + Danishefsky diene (Product - exo)

Fe	2.22736	0.62397	-1.31400
C	3.25426	-0.53544	-2.22117
C	2.61822	0.19207	0.36184
C	3.34209	2.00685	-1.57987
C	0.57955	0.25324	-2.46628
C	0.62631	1.62036	-2.10949
C	0.66324	1.86144	-0.70053
C	-0.29118	1.11417	0.21149
C	-0.34559	-0.38364	-0.17263
C	0.57610	-0.64575	-1.35220
H	0.66153	-0.07124	-3.50595
H	0.74783	2.40473	-2.85967
H	0.86454	2.89137	-0.39023
H	0.09443	1.17704	1.23955
H	0.03264	-0.96348	0.68340
H	0.71604	-1.70695	-1.58699
O	2.81468	-0.08796	1.45324
O	3.87946	-1.30462	-2.78861
O	4.02537	2.90987	-1.72602
C	-2.75894	-0.37981	0.56909
H	-2.09267	-0.56736	-1.45099
C	-1.77169	-0.89926	-0.44703
H	-1.77409	-1.99902	-0.47313
C	-2.70450	0.91366	0.90660
H	-3.44535	1.35366	1.57708
C	-1.68159	1.79369	0.23255
O	-1.63535	3.09728	0.76436
O	-3.71490	-1.21510	1.03197
C	-1.21359	3.22672	2.09128
H	-1.50813	4.22920	2.43114
H	-0.11614	3.13934	2.20061
H	-1.68306	2.48131	2.75926
H	-1.98577	1.95406	-0.81832
Si	-3.51807	-2.64934	1.91051
C	-4.95064	-2.69818	3.10642
H	-5.90865	-2.65399	2.56576
H	-4.93793	-3.62504	3.70154
H	-4.91339	-1.84371	3.79917

C	-3.59685	-4.11229	0.74225
H	-2.74479	-4.13265	0.04553
H	-3.59058	-5.05895	1.30631
H	-4.52156	-4.08111	0.14519
C	-1.86838	-2.57260	2.79554
H	-1.78687	-1.64766	3.38765
H	-1.74843	-3.42796	3.47916
H	-1.02688	-2.59218	2.08526

Electronic energy (a.u.) at ωB97X-D/def2-SVP: –2589.1623904
Gibbs free energy correction (a.u.) at ωB97X-D/def2-SVP: 0.303967
Electronic energy (a.u.) at ωB97X-D/def2-TZVPP: –2590.5980573
Electronic energy (a.u.) at DLPNO-CCSD(T)/def2-TZVPP: –2587.64814
Number of imaginary frequencies: 0