



Supporting Information

for

Computational characterization of enzyme-bound thiamin diphosphate reveals a surprisingly stable tricyclic state: implications for catalysis

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Lowest-energy conformation of model A, superpositions of the AP state/model C and APH⁺ state/model E with crystal structures, superposition of the AP state/models B and C, superposition of the AP states/models D and E, experimental CD spectra, calculated energies and energy corrections, and Cartesian coordinates of all optimized structures

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1. Lowest-energy structure of the cofactor alone

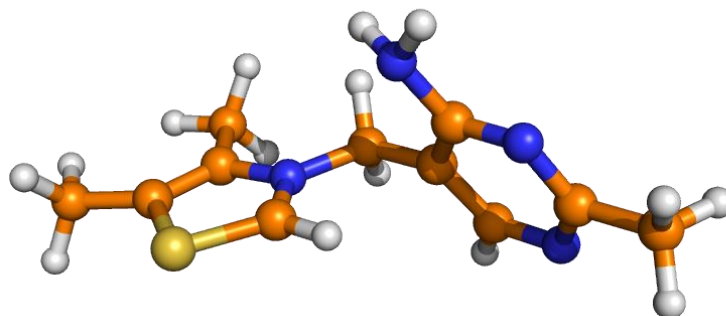
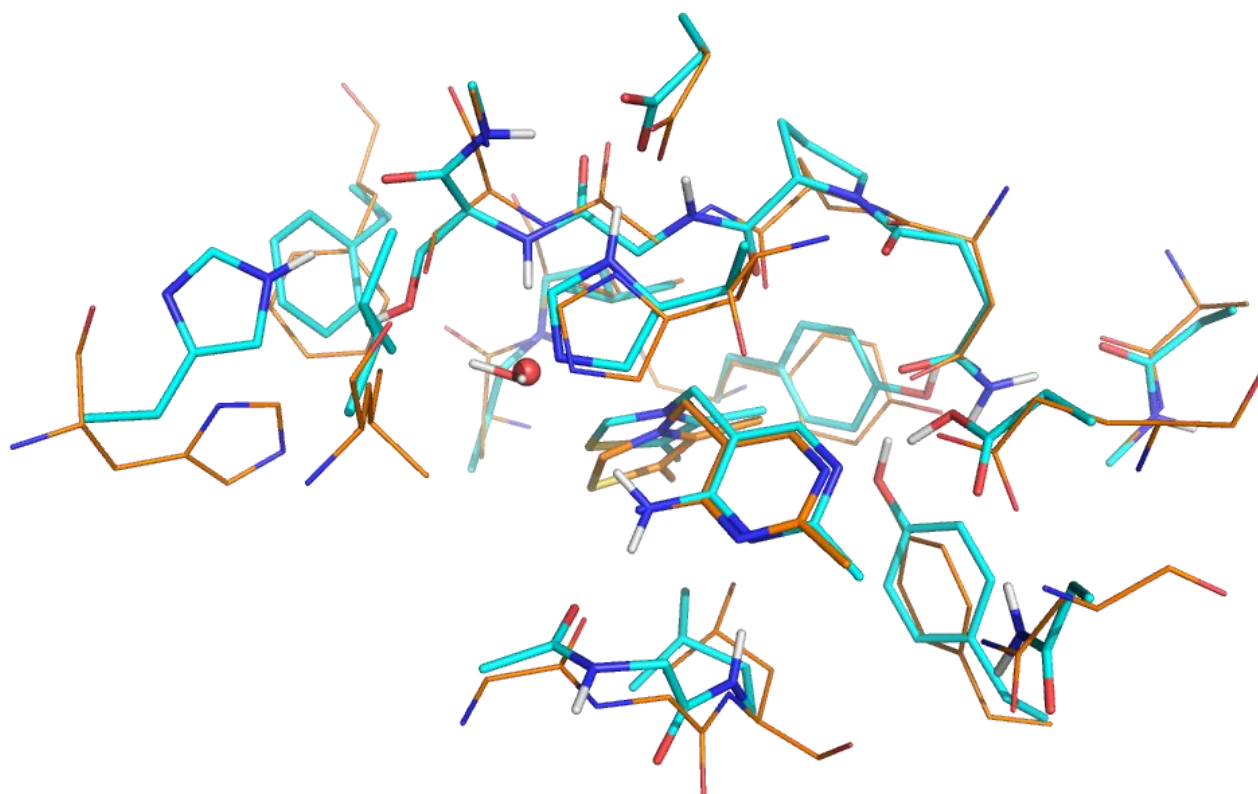


Figure S1: *Lowest-energy conformation of the cofactor alone in solution (Model A). This structure is calculated to be 4.2 kcal/mol lower in energy than the typical V-shape of the AP state shown in Figure 2 in the main text.*

2. Superposition of AP state in Model C with crystal structure



*Figure S2: Residues colored in orange and the water represented as a sphere correspond to the crystal structure containing the crystallographic water (PDB 1BFD). Residues in turquoise and the water represented with lines correspond to the AP state of **Model C**.*

3. Superposition of APH⁺ state in Model E with crystal structure

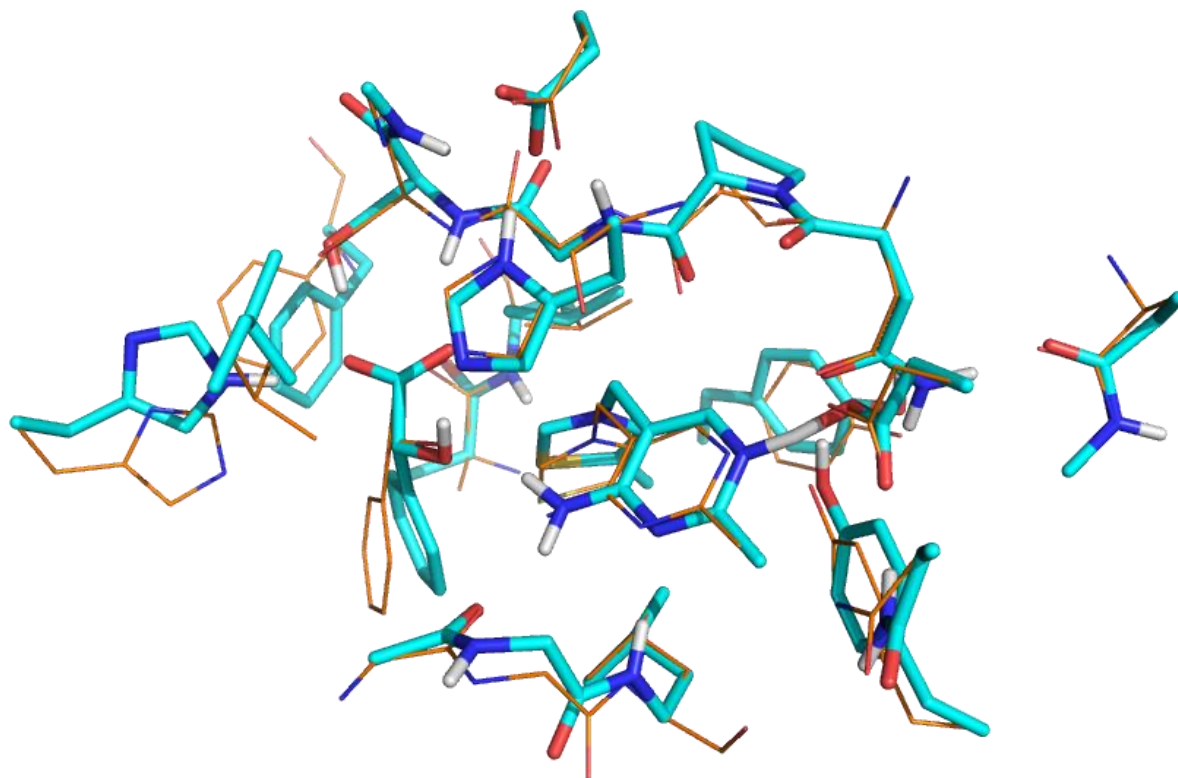


Figure S3: Residues colored in orange correspond to the crystal structure containing R-Mandelate (PDB 1MCZ), while residues colored in turquoise correspond to the APH⁺ state of Model E.

4. Superposition of the AP states for Models B and C

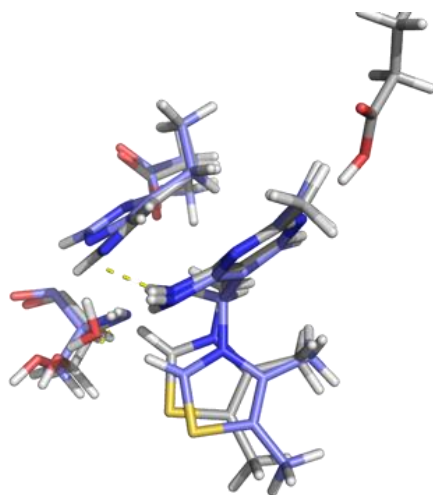


Figure S4: Superposition of the AP states of **Model B** representing the empty cavity (grey color) with **Model C** that includes the crystallographic water (blue color).

5. Superposition of the AP states for Models D and E

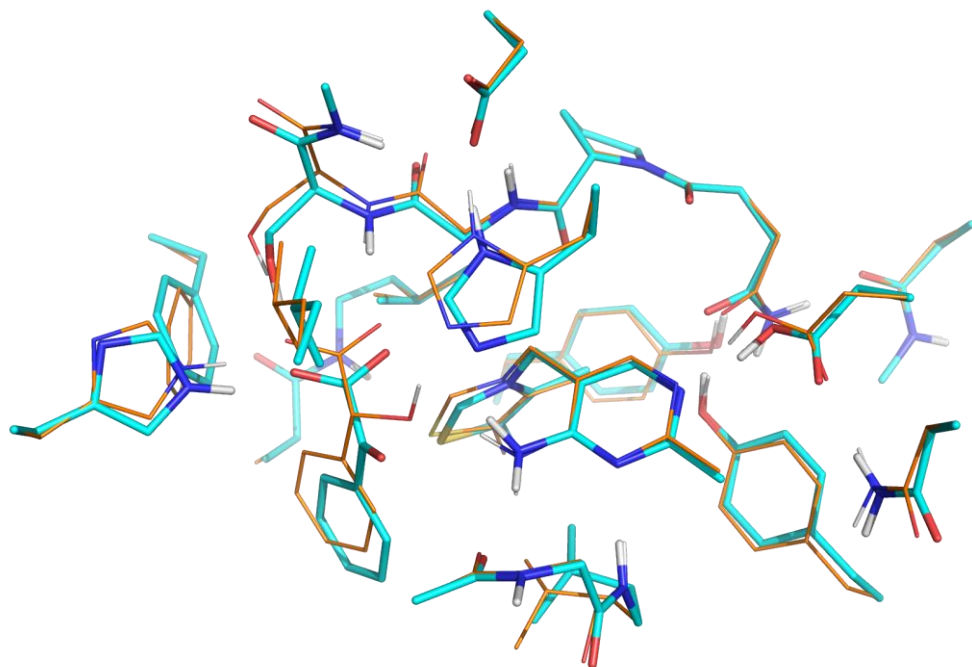


Figure S5: Superposition of the AP states of Model D representing the active site with benzoylformate substrate (blue color) with Model E that includes the (R)-mandelate inhibitor (orange color).

6. Experimental CD spectra

Aliquots of (*R*)-mandelate or methyl benzoyl phosphonate (MBP) were added to BFDC (2.0 mg/mL, 35 μ M concentration of active centers) in 20 mM KH_2PO_4 (pH 6.5), containing MgCl_2 (2.5 mM) and ThDP (0.50 mM). The CD spectra were recorded in the near-UV region using a Jasco J-810 circular dichroism spectropolarimeter. Difference spectra were obtained by subtraction of the spectrum of BFDC in the absence of ligand using SigmaPlot 12.

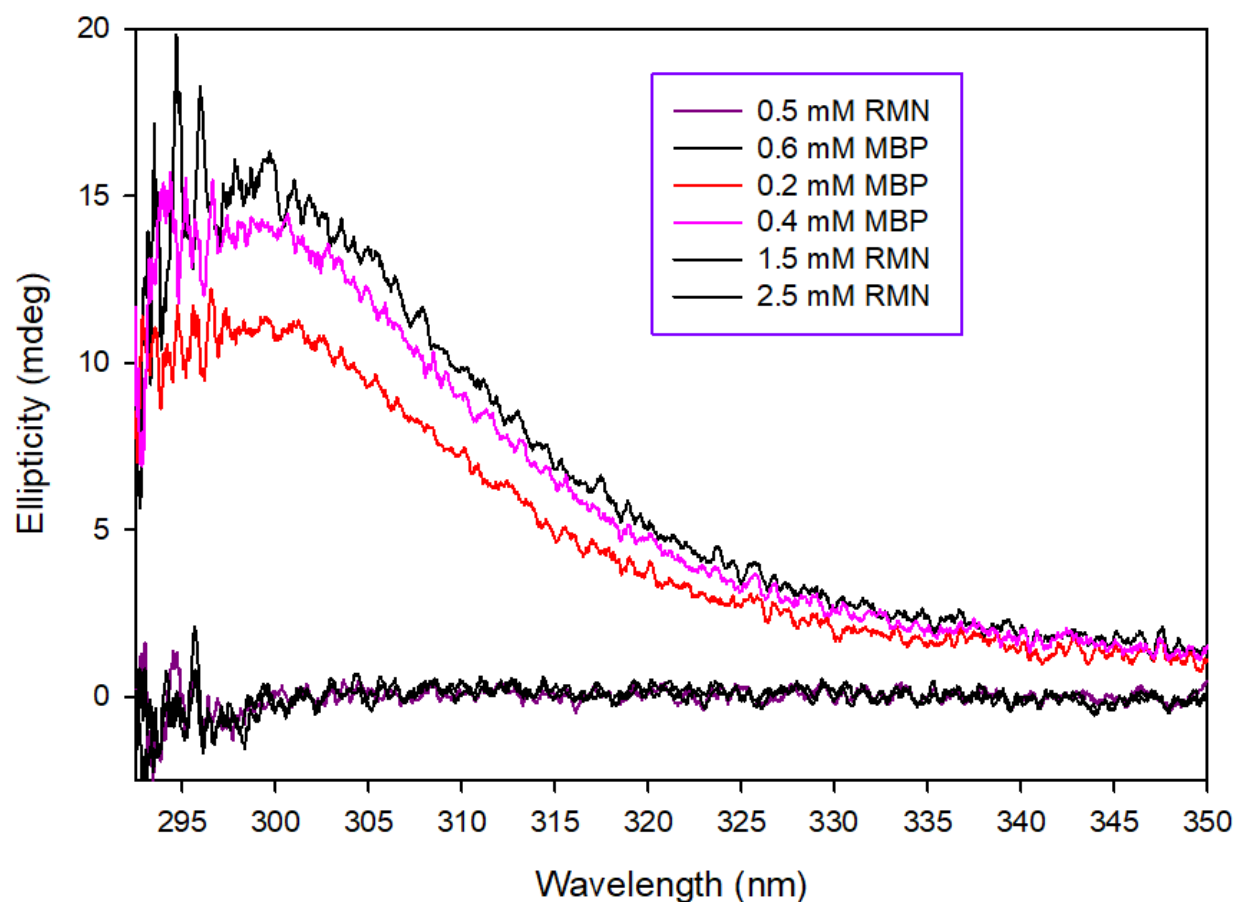


Figure S6: Titration of BFDC (2 mg/mL) with methyl benzoyl phosphonate and *R*-mandelate at pH 6.5. Difference spectra were obtained by subtracting the spectra of BFDC in the absence of ligand.

7. Energy decomposition of the calculated stationary points

	State	E_{el} (a.u.)	E_{bb} (a.u.)	E_{solv} (a.u.)	ZPE (a.u.)	E_{tot} (a.u.)	E_{rel} (kcal/mol)
Cofactor alone (Model A)	AP	-1045.28221	-1045.47855	-1045.35311	0.20993	-1045.33951	0.0
	IP	-1045.27665	-1045.47334	-1045.34318	0.21059	-1045.32928	7.4
	YIH ⁺	-1045.26352	-1045.45822	-1045.33111	0.21056	-1045.31526	15.6
	TCH ⁺	-1045.28181	-1045.47440	-1045.35747	0.21505	-1045.33502	2.9
Empty Cavity (Model B)	AP	-6380.26084	-6381.95241	-6380.34894	2.51861	-6379.54903	0.0
	APH ⁺ a	-6380.25933	-6381.95903	-6380.37001	2.52255	-6379.54715	1.2
	IP	-6380.23940	-6381.94395	-6380.34264	2.51862	-6379.52857	12.8
	YI	-6380.25425	-6381.95597	-6380.34900	2.52024	-6379.53048	11.6
	YIH ⁺ a	-6380.25170	-6381.95242	-6380.34895	2.51861	-6379.53105	11.3
	TC	-6380.27087	-6381.97007	-6380.36693	2.52131	-6379.54483	2.6
	TCH ⁺ a	-6380.26542	-6381.96515	-6380.36540	2.51928	-6379.54585	2.0
Crystallographic water (Model C)	AP	-6456.72502	-6458.45660	-6456.82834	2.54663	-6456.01329	0.0
	APH ⁺ a	-6456.71750	-6458.44888	-6456.82408	2.54513	-6456.01032	1.9
	IP	-6456.69510	-6458.42979	-6456.79865	2.54562	-6455.98772	16.0
	YI	-6456.72457	-6458.45349	-6456.81461	2.54778	-6455.99576	11.0
	YIH ⁺ a	-6456.71868	-6458.44791	-6456.81255	2.54625	-6455.99553	11.1
	TC	-6456.72875	-6458.45789	-6456.81906	2.54904	-6455.99916	8.9
	TCH ⁺ a	-6913.97667	-6915.84279	-6914.10174	2.61823	-6913.33804	8.5
Benzoylformate (Model D)	AP	-6913.99977	-6915.86226	-6914.13179	2.63767	-6913.35662	0.0
	APH ⁺	-6913.98709	-6915.85037	-6914.12303	2.63451	-6913.35180	3.0
	IP	-6914.00520	-6915.86876	-6914.13032	2.63584	-6913.35804	-0.9
	YI	-6914.00338	-6915.86418	-6914.12611	2.63507	-6913.35183	3.0
	YIH ⁺	-6914.00856	-6915.86697	-6914.12503	2.63632	-6913.34713	6.0
	TC	-6914.02630	-6915.88361	-6914.14442	2.63727	-6913.36446	-4.9
	TCH ⁺	-6914.02416	-6915.88291	-6914.14564	2.63779	-6913.36660	-6.3
R-Mandelate (Model E)	AP	-6915.23515	-6917.09728	-6915.36515	2.66107	-6914.56621	0.0
	APH ⁺	-6915.23045	-6917.09363	-6915.36243	2.65900	-6914.56661	-0.3
	IP	-6915.22148	-6917.08475	-6915.34650	2.65985	-6914.54993	10.2

	YI	-6915.21059	-6917.07054	-6915.32913	2.65988	-6914.52920	23.2
	YIH⁺	-6915.20512	-6917.06794	-6915.33055	2.65936	-6914.53401	20.2
	TC	-6915.23856	-6917.09747	-6915.35729	2.66259	-6914.55361	7.9
	TCH⁺	-6915.22551	-6917.08637	-6915.34831	2.66092	-6914.54825	11.3

^aThese states have the N1'-H bond restrained to 1.15 Å in the geometry optimization.

E_{el} = Energy of the optimized geometry at B3LYP/6-31G(d,p) level.

E_{bb} = Single-point energy of the optimized geometry at B3LYP/6-311+G(2d,2p) level.

E_{solv} = Single-point energy of the optimized geometry at B3LYP/6-31G(d,p) and SMD solvation method with $\epsilon = 4$

$E_{\text{tot}} = E_{\text{bb}} + (E_{\text{solv}} - E_{\text{el}}) + \text{ZPE}$

E_{rel} = Energy relative to **AP** in each respective model

All calculations include empirical dispersion according to Grimme's D3(BJ) method.

8. Cartesian coordinates of optimized structures

Cofactor alone Model A

AP

C	1.7589	1.5106	0.0781
C	1.2530	0.4114	0.7730
C	2.0354	-0.7595	0.6971
N	1.6526	-1.9482	1.3110
N	3.1485	-0.8083	-0.0387
C	3.5212	0.3019	-0.6920
N	2.8721	1.4817	-0.6467
S	-2.5493	-1.5611	-0.7980
C	-1.1872	-1.2410	0.1524
C	4.7656	0.2389	-1.5215
N	-1.1972	-0.0079	0.6446
C	-2.3125	0.7586	0.2802
C	-2.4646	2.1683	0.7549
C	-0.0608	0.4934	1.4908
H	-0.3720	-1.9328	0.3478
H	2.3827	-2.6495	1.2333
H	-0.2920	1.5259	1.7431
H	-0.0892	-0.0804	2.4203
H	4.5587	0.6002	-2.5327
H	5.5242	0.9047	-1.0971
H	5.1551	-0.7777	-1.5575
H	1.2286	2.4633	0.1129
H	-2.4876	2.2254	1.8476
H	-1.6532	2.8060	0.3903
H	-3.4009	2.5857	0.3870
C	-3.1677	0.0513	-0.5219
C	-4.4706	0.4687	-1.1282
H	-5.3073	-0.0652	-0.6670
H	-4.6356	1.5378	-0.9904
H	-4.4896	0.2640	-2.2021
H	1.3121	-1.8670	2.2624

IP

C	-1.9121	1.3430	-0.5982
C	-1.2056	0.2075	-0.8043
C	-1.7469	-1.0614	-0.2980
N	-1.1146	-2.1624	-0.5238
N	-2.9562	-1.0228	0.4085
C	-3.5775	0.0960	0.5813
N	-3.0934	1.3000	0.0971
S	2.9870	-1.4196	0.4860
C	1.6249	-1.3539	-0.5190
C	-4.8777	0.1560	1.3234
N	1.2610	-0.1066	-0.7841
C	2.0593	0.8793	-0.1853
C	1.7604	2.3278	-0.3965
C	0.0525	0.1812	-1.6150
H	1.0061	-2.1878	-0.8367
H	-1.6425	-2.9406	-0.1238
H	0.2320	1.1249	-2.1286
H	-0.0006	-0.6173	-2.3569
H	-4.8015	0.8194	2.1916
H	-5.6761	0.5366	0.6771
H	-5.1396	-0.8455	1.6596
H	-1.6100	2.3146	-0.9729
H	1.8453	2.6086	-1.4513
H	0.7523	2.5760	-0.0520
H	-3.6328	2.1433	0.2309
H	2.4646	2.9421	0.1630

C	3.0689	0.3300	0.5532
C	4.1559	1.0021	1.3311
H	5.1337	0.8304	0.8705
H	3.9901	2.0793	1.3752
H	4.1965	0.6273	2.3577

YIH⁺

C	1.9316	1.4317	0.3610
C	1.2029	0.3262	0.6698
C	1.7944	-0.9508	0.3130
N	1.1596	-2.0844	0.5186
N	3.0483	-1.0121	-0.2340
C	3.6968	0.0864	-0.5007
N	3.1551	1.3168	-0.2399
S	-2.9106	-1.5272	-0.3590
C	-1.4712	-1.3379	0.5430
C	5.0638	0.0461	-1.1054
N	-1.2784	-0.0135	0.6934
C	-2.2176	0.8802	0.1275
C	-2.0562	2.3604	0.2686
C	-0.0901	0.4311	1.4446
H	1.6400	-2.9295	0.2308
H	-0.2397	1.4587	1.7742
H	-0.0252	-0.1957	2.3374
H	5.0790	0.5730	-2.0653
H	5.7939	0.5248	-0.4442
H	5.3518	-0.9916	-1.2634
H	1.6005	2.4385	0.5866
H	-2.1107	2.6820	1.3147
H	-1.1032	2.7075	-0.1468
H	-2.8508	2.8770	-0.2697
C	-3.2133	0.2010	-0.5014
C	-4.4244	0.7234	-1.2068
H	-5.3400	0.4392	-0.6784
H	-4.4028	1.8129	-1.2753
H	-4.4916	0.3249	-2.2235
H	0.0907	-2.0697	0.6822
H	3.6857	2.1500	-0.4612

TCH⁺

C	-2.2195	1.5196	-0.3289
C	-1.1279	0.8355	-0.7562
C	-1.1128	-0.5766	-0.4859
N	-0.0730	-1.3061	-0.8683
N	-2.1413	-1.2057	0.1431
C	-3.1803	-0.4999	0.5111
N	-3.2402	0.8486	0.2950
S	2.5939	-1.4650	-0.3676
C	1.2384	-0.7096	-1.3185
C	-4.3483	-1.1496	1.1806
N	1.2830	0.6978	-1.0241
C	1.8008	0.9279	0.2945
C	1.5973	2.2748	0.9090
C	2.5243	-0.0916	0.7867
C	3.3107	-0.1981	2.0518
C	0.0819	1.4065	-1.4568
H	1.3511	-0.9141	-2.3846
H	-0.0847	-2.2903	-0.6174
H	-0.0164	1.2774	-2.5409
H	-4.5939	-0.6453	2.1206
H	-5.2310	-1.1090	0.5329
H	-2.3483	2.5878	-0.4582
H	1.9734	3.0648	0.2488
H	2.1353	2.3500	1.8532
H	0.5402	2.4842	1.1147
H	3.2269	0.7140	2.6454
H	4.3737	-0.3635	1.8432
H	2.9627	-1.0354	2.6659
H	0.1886	2.4753	-1.2689
H	-4.1080	-2.1918	1.3830
H	-4.0598	1.3597	0.5997

Empty cavity

Model B

AP

C	11.5114	5.5184	-1.5740
C	10.8579	4.1408	-1.7482
C	10.0720	3.6562	-0.5625
C	9.7913	4.2941	0.6237
N	9.5102	2.3878	-0.5509
C	8.9016	2.2671	0.6154
N	9.0437	3.3951	1.3627
H	10.7588	6.2925	-1.3886
H	11.6280	3.3935	-1.9779
H	10.1973	4.1557	-2.6254
H	10.0423	5.2727	0.9999
H	8.3502	1.4118	0.9818
H	8.6371	3.5461	2.2724
C	-9.4680	1.9224	-4.3238
C	-8.3756	2.6355	-3.5072
C	-7.2895	1.7008	-3.0226
C	-6.2428	1.3057	-3.8687
C	-7.2957	1.4830	-1.7227
C	-5.2458	0.4345	-3.4383
C	-6.3038	0.3121	-1.2720
C	-5.2628	-0.0687	-2.1303
O	-4.2556	-0.9010	-1.7670
H	-9.9588	1.1505	-3.7221
H	-8.8348	3.1368	-2.6468
H	-7.9299	3.4253	-4.1246
H	-6.2011	1.6955	-4.8830
H	-8.0760	1.4909	-1.0309
H	-4.4350	0.1421	-4.0970
H	-6.3157	-0.0306	-0.2457
H	-4.3044	-1.1755	-0.8170
C	-0.1697	-6.7752	-5.1636
C	-0.1913	-6.5664	-3.6457
C	-1.4157	-5.8771	-3.0778
C	-1.7712	-6.1039	-1.7421
C	-2.2052	-4.9838	-3.8150
C	-2.8640	-5.4721	-1.1584
C	-3.3110	-4.3483	-3.2492
C	-3.6469	-4.5985	-1.9174
O	-4.7614	-3.9970	-1.4070
H	-0.1524	-5.8231	-5.7038
H	-0.0805	-7.5371	-3.1479
H	0.7026	-5.9913	-3.3637
H	-1.1819	-6.7941	-1.1448
H	-1.9654	-4.7812	-4.8540
H	-3.1179	-5.6659	-0.1191
H	-3.9155	-3.6500	-3.8170
H	-4.7670	-4.0981	-0.4455
C	4.9875	-4.3007	-5.9139
C	4.5141	-4.1976	-4.4739
O	4.2960	-3.1148	-3.9253
C	4.4778	-3.1495	-6.7791
H	6.0851	-4.2828	-5.8747
H	4.7222	-2.1949	-6.3088
H	3.3903	-3.1969	-6.8942
H	4.9267	-3.1786	-7.7751
N	4.4213	-5.3883	-3.8260
C	4.5262	-5.5148	-2.3752
C	3.2237	-5.5889	-1.5809
C	2.5060	-4.2505	-1.3581
C	1.2739	-4.4732	-0.4763
C	3.4432	-3.2114	-0.7329
H	4.6496	-6.2096	-4.3658
H	5.1287	-4.6833	-2.0077
H	3.4752	-6.0047	-0.5953
H	2.5464	-6.3087	-2.0571
H	2.1837	-3.8722	-2.3345
H	1.5739	-4.8138	0.5221
H	0.6930	-3.5608	-0.3346
H	0.6020	-5.2219	-0.9039
H	4.2501	-2.9277	-1.4088
H	3.8673	-3.5831	0.2057
H	2.8959	-2.2975	-0.5014

C 9.5105 -5.2180 -1.3683
C 8.2681 -4.4440 -0.9044
C 8.2305 -3.0069 -1.3793
C 7.2467 -2.5633 -2.2693
C 9.1677 -2.0760 -0.9085
C 7.1732 -1.2230 -2.6573
C 9.1103 -0.7395 -1.2980
C 8.1040 -0.3042 -2.1674
H 10.4281 -4.7388 -1.0154
H 8.2275 -4.4585 0.1923
H 7.3674 -4.9634 -1.2496
H 6.5141 -3.2606 -2.6573
H 9.9360 -2.3979 -0.2101
H 6.3865 -0.9146 -3.3401
H 9.8209 -0.0102 -0.9243
H 8.0747 0.7443 -2.4485
C -2.5742 0.8441 0.4263
C -1.3164 1.1261 -0.0707
C -1.1889 2.3320 -0.8187
N 0.0024 2.8015 -1.2504
N -2.2938 3.0411 -1.1477
C -3.4728 2.6646 -0.6434
N -3.6466 1.6182 0.1808
S 2.4318 -0.3743 -2.6324
C 1.7921 0.2732 -1.2065
C -4.6820 3.4627 -1.0199
N 0.5991 -0.2318 -0.9163
C 0.1251 -1.1822 -1.8255
C -1.1930 -1.8467 -1.6162
C 1.0163 -1.3758 -2.8473
C 0.8901 -2.2641 -4.0433
C -0.1684 0.2237 0.2728
H 2.2882 1.0019 -0.5743
H 0.0289 3.6924 -1.7504
H -0.5190 -0.6702 0.7929
H 0.5448 0.7335 0.9163
H -5.1527 3.0155 -1.9016
H -5.4046 3.4421 -0.2054
H -4.4097 4.4910 -1.2599
H -2.7485 -0.0299 1.0503
H -1.2993 -2.1973 -0.5856
H -1.2830 -2.7102 -2.2741
H -2.0259 -1.1724 -1.8369
H 0.2469 -3.1169 -3.8129
H 1.8705 -2.6351 -4.3513
C 2.4643 -2.4817 7.1084
C 1.6856 -1.1650 6.9822
C 2.3851 -0.1470 6.0707
O 2.5390 -0.5259 4.8326
O 2.7525 0.9427 6.5212
C -7.9311 2.7694 4.0749
C -7.1059 1.6026 3.5436
C -6.3667 1.9308 2.2624
O -6.5300 2.9754 1.6407
O -5.5277 0.9777 1.9000
H -8.4282 2.4921 5.0090
H -7.2997 3.6388 4.2703
H -7.7342 0.7247 3.3440
H -6.3587 1.2692 4.2724
C -0.3642 2.1749 5.1491
C -0.2904 1.5609 3.7494
C 0.8817 2.0086 2.9344
C 0.9413 2.8431 1.8373
N 2.1604 1.5098 3.0747
C 2.9118 2.0149 2.0567
N 2.2006 2.8209 1.2681
H 0.5374 1.9541 5.7279
H -0.2754 0.4682 3.8244
H -1.1975 1.8099 3.1875
H 0.1379 3.4315 1.4186
H 3.9688 1.8166 1.9459
C 5.6882 7.3426 2.1978
C 5.3352 6.1081 3.0354
C 6.0498 4.8114 2.6109
C 5.8067 3.6981 3.6406
C 5.6440 4.3511 1.2049
H 5.3842 7.2241 1.1523

H 4.2510 5.9353 3.0009
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TCH⁺

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H	-4.2671	2.1419	-3.8822	H	-11.3083	-4.3462	4.7231	H	4.8140	-3.7659	-7.4799
H	-4.1029	1.9438	-5.6114	H	-11.2459	-3.1044	3.4621	N	4.0508	-5.6598	-3.4226
H	-1.8269	1.9415	-3.5745	H	-11.4172	-5.4092	2.4286	C	4.2784	-5.8264	-1.9976
H	-0.3389	1.2684	-5.4348	H	-8.7192	-4.1829	-0.9574	C	3.0460	-5.6494	-1.1128
H	-1.6531	1.5250	-6.5981	H	-6.7910	6.1569	1.8258	C	2.4816	-4.2248	-1.0547
H	-0.9756	2.8909	-5.6927	H	-8.2258	5.1608	1.8854	C	1.2232	-4.2121	-0.1828
H	-3.0370	-0.3212	-5.2331	H	-8.1156	4.5475	-0.2528	C	3.5210	-3.2173	-0.5464
H	-3.2305	-0.0921	-3.4942	H	-8.3709	5.6852	-1.5738	H	3.7241	-6.4620	-3.9407
H	-1.6374	-0.4614	-4.1531	H	-9.5922	7.1302	2.6541	H	5.0506	-5.1097	-1.7188
H	-2.8762	4.0999	-5.8128	H	-8.1887	6.9439	3.7196	H	3.3237	-5.9616	-0.0968
C	-4.5264	-2.9138	3.9026	H	-8.1972	8.1874	2.4453	H	2.2592	-6.3419	-1.4420
C	-3.1220	-2.2843	3.9075	H	-9.9451	-5.8926	3.2821	H	2.2023	-3.9402	-2.0780
O	-2.9507	-1.0685	3.8271	H	-8.9959	-2.6224	-0.1640	H	1.4585	-4.5334	0.8385
C	-5.5306	-2.0802	3.0804	H	-10.2066	-3.2692	-1.2908	H	0.7775	-3.2212	-0.1015
C	-5.2792	-2.1771	1.5836	H	-11.1461	-4.4500	0.4525	H	0.4526	-4.8806	-0.5785
N	-6.1435	-2.9199	0.8719					H	4.3851	-3.1539	-1.2122
O	-4.3039	-1.6129	1.0489					H	3.8618	-3.4851	0.4604
N	-2.0727	-3.1340	4.0952					H	3.0942	-2.2133	-0.4850
C	-0.7213	-2.6130	4.2693					C	9.2782	-5.5605	-1.0628
C	-0.0569	-2.2725	2.9260					C	8.1134	-4.5599	-0.9587
O	-0.4211	-2.7918	1.8729					C	8.5092	-3.1069	-1.1411
C	0.0224	-3.8013	4.9134					C	7.8913	-2.3140	-2.1168
C	-0.6380	-5.0107	4.2355					C	9.4903	-2.5185	-0.3284
C	-2.1155	-4.6022	4.1159					C	8.2472	-0.9703	-2.2744
N	0.9932	-1.4215	3.0414					C	9.8520	-1.1823	-0.4909
C	1.9340	-1.1822	1.9718					C	9.2305	-0.3963	-1.4666
C	3.3698	-1.3696	2.4530					H	10.0393	-5.3711	-0.3003
O	3.6478	-2.0196	3.4654					H	7.6294	-4.6811	0.0205
N	4.3146	-0.7695	1.6899					H	7.3544	-4.8073	-1.7081
C	5.7438	-0.9026	1.9591					H	7.1267	-2.7464	-2.7561
C	6.2280	0.1129	3.0261					H	9.9768	-3.1132	0.4402
O	6.9921	1.0448	2.7509					H	7.7607	-0.3764	-3.0437
C	6.5320	-0.8024	0.6639					H	10.6185	-0.7435	0.1388
O	6.1268	0.3727	-0.0413					H	9.5252	0.6406	-1.5940

**Crystallographic water
Model C**

AP

C	11.4992	5.0827	-2.1138
C	10.3586	4.0471	-2.2260
C	10.0056	3.3124	-0.9564
C	8.7614	3.1269	-0.3840
N	10.9605	2.6449	-0.2080
C	10.3037	2.0831	0.7911
N	8.9664	2.3378	0.7354
H	11.2279	5.8935	-1.4305
H	10.6449	3.3065	-2.9857
H	9.4529	4.5354	-2.6053
H	7.7823	3.4923	-0.6475

C -2.5090 0.8338 0.3037
 C -1.2950 1.0253 -0.3296
 C -1.1891 2.1795 -1.1515
 N -0.0251 2.5629 -1.7066
 N -2.2840 2.9297 -1.4125
 C -3.4301 2.6234 -0.7965
 N -3.5742 1.6320 0.1005
 S 1.8464 -1.2364 -3.2048
 C 1.5309 -0.3016 -1.8293
 C -4.6380 3.4383 -1.1402
 N 0.3560 -0.5954 -1.2852
 C -0.3568 -1.6151 -1.9335
 C -1.6609 -2.1000 -1.4038
 C 0.3224 -2.0711 -3.0295
 C -0.0785 -3.1284 -4.0059
 C -0.1358 0.1178 -0.0663
 H 2.2574 0.3924 -1.3872
 H 0.0439 3.4368 -2.2355
 H -0.4018 -0.6505 0.6632
 H 0.7181 0.6760 0.3210
 H -5.2006 2.9353 -1.9342
 H -5.2870 3.5252 -0.2702
 H -4.3489 4.4270 -1.4975
 H -2.6514 0.0161 1.0063
 H -1.6164 -2.2520 -0.3218
 H -1.9134 -3.0538 -1.8659
 H -2.4707 -1.4018 -1.6274
 H -0.8611 -3.7587 -3.5819
 H 0.7700 -3.7697 -4.2634
 C 2.3831 -2.0297 7.2426
 C 1.6412 -0.6904 7.2453
 C 2.3087 0.3021 6.2904
 O 2.3434 -0.0838 5.0491
 O 2.7759 1.3672 6.7073
 C -7.9334 3.1954 3.9097
 C -7.0569 2.0066 3.5304
 C -6.2616 2.2395 2.2634
 O -6.3310 3.2728 1.6078
 O -5.4849 1.2135 1.9535
 H -8.4755 2.9897 4.8374
 H -7.3321 4.0943 4.0577
 H -7.6507 1.0954 3.3857
 H -6.3361 1.7639 4.3201
 C -0.3692 2.5224 4.9566
 C -0.3026 1.8797 3.5628
 C 0.9599 2.2240 2.8416
 C 1.2159 2.8947 1.6629
 N 2.2009 1.9088 3.3563
 C 3.1316 2.3754 2.4994
 N 2.5828 2.9825 1.4497
 H 0.4943 2.2451 5.5663
 H -0.3942 0.7923 3.6630
 H -1.1530 2.2021 2.9524
 H 0.5075 3.3373 0.9773
 H 4.1892 2.2346 2.6577
 H 0.8438 2.2017 -1.3495
 C 5.7566 7.3164 1.5598
 C 5.6908 6.3223 2.7206
 C 6.3716 4.9678 2.4547
 C 6.2830 4.0826 3.7043
 C 5.7696 4.2636 1.2299
 H 5.2156 6.9480 0.6825
 H 4.6395 6.1341 2.9790
 H 6.1474 6.7754 3.6102
 H 7.4363 5.1553 2.2483
 H 5.2376 3.8804 3.9652
 H 6.7850 3.1222 3.5555
 H 6.7423 4.5758 4.5683
 H 4.6773 4.2412 1.2846
 H 6.1162 3.2267 1.1583
 H 6.0407 4.7743 0.3000
 H -0.4634 -2.6829 -4.9295
 H -8.6627 3.4079 3.1270
 H 12.4032 4.6061 -1.7261
 H 11.7213 5.5152 -3.0939
 H -10.3493 2.3926 -4.8049
 H -9.1029 1.1976 -5.2080

H -0.3805 3.6139 4.8778
 H -1.2779 2.2043 5.4766
 H 6.7940 7.5004 1.2559
 H 5.3160 8.2793 1.8381
 H 0.6052 -0.8407 6.9120
 H 1.6121 -0.2539 8.2467
 H 2.4763 -2.4113 6.2221
 H 1.8726 -2.7809 7.8552
 H 3.3964 -1.9089 7.6409
 H 8.9198 -6.5861 -0.9292
 H 9.7642 -5.4903 -2.0408
 H 4.6943 -6.8289 -1.8348
 H 0.4504 -7.7128 -4.9152
 H -1.3141 -7.8425 -4.9049
 H 3.9432 -5.5978 -5.9401
 H 2.3731 1.2285 4.1548
 H -4.8531 1.4261 1.1789
 C 2.1241 6.5259 -4.0059
 C 0.9090 5.9250 -3.3480
 O 0.7861 4.7028 -3.2303
 N -0.0368 6.7982 -2.9136
 C -1.3721 6.2993 -2.6401
 C -2.0179 5.7983 -3.9433
 O -1.8151 6.3865 -5.0030
 N -2.8070 4.7131 -3.7860
 C -3.4133 4.0359 -4.9223
 C -3.0285 2.5521 -4.9545
 C -1.5169 2.2768 -4.9502
 C -1.2515 0.7742 -4.8032
 C -0.8086 2.8629 -6.1757
 H 2.9996 5.9245 -3.7588
 H 1.9806 6.4898 -5.0910
 H -1.3260 5.5119 -1.8852
 H -1.9715 7.1191 -2.2360
 H -3.4808 2.0548 -4.0887
 H -3.4877 2.0972 -5.8436
 H -1.0921 2.7666 -4.0704
 H 0.2633 2.6421 -6.1433
 H -1.2121 2.4421 -7.1054
 H -0.9170 3.9502 -6.2162
 H -1.6442 0.2151 -5.6621
 H -1.7271 0.3752 -3.8999
 H -0.1773 0.5720 -4.7360
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 C -4.6834 -2.7960 3.8241
 C -3.2850 -2.1520 3.9114
 O -3.1531 -0.9346 4.0099
 C -5.6625 -1.9306 3.0178
 C -5.3892 -1.9644 1.5284
 N -6.3532 -2.4882 0.7434
 O -4.3305 -1.5256 1.0452
 N -2.2186 -2.9984 3.9715
 C -0.8690 -2.5017 4.2308
 C -0.1529 -2.0632 2.9418
 O -0.6119 -2.3406 1.8222
 C -0.1619 -3.7466 4.8038
 C -0.7731 -4.8768 3.9623
 C -2.2444 -4.4566 3.7977
 N 1.0272 -1.4553 3.1475
 C 1.9295 -1.1445 2.0663
 C 3.3787 -1.4545 2.4270
 O 3.7021 -2.3615 3.1915
 N 4.2670 -0.6359 1.8079
 C 5.7012 -0.7671 2.0060
 C 6.2452 0.1310 3.1489
 O 7.2673 0.8140 2.9975
 C 6.4775 -0.6034 0.7124
 O 6.2445 0.6894 0.1206
 N 5.5509 0.0299 4.2998
 C 5.9530 0.6223 5.5736
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 H -5.5349 -0.8888 3.3234
 H -4.6464 -3.8108 3.4207
 H -0.4220 -3.8592 5.8611
 H 0.9238 -3.6813 4.7179
 H -0.6747 -5.8621 4.4236
 H -0.2895 -4.9067 2.9821

H -2.8798 -4.9267 4.5584
 H -2.6333 -4.7283 2.8103
 H -0.9072 -1.6644 4.9311
 H 1.8613 -0.0908 1.7931
 H 1.6499 -1.7483 1.2015
 H 7.5404 -0.7159 0.9276
 H 6.1758 -1.3914 0.0146
 H 6.9742 0.8415 -0.4977
 H 5.8623 -1.8004 2.3388
 H 6.7561 1.3335 5.3833
 H 2.2963 7.5643 -3.7124
 H -4.5063 4.1229 -4.8681
 H -2.6803 4.1704 -2.9297
 H 0.0142 7.7331 -3.2921
 H 6.3168 -0.1545 6.2557
 H 5.0942 1.1270 6.0246
 H 4.7186 -0.5504 4.3191
 H 1.3483 -1.1228 4.0786
 H -7.2127 -2.8961 1.1164
 H -6.2025 -2.4792 -0.2575
 H 3.9293 0.0781 1.1636
 H -5.0506 -2.8804 4.8537
 C -10.5336 -4.8627 2.6728
 C -9.6757 -4.2335 1.5982
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 N -10.2534 -4.0459 0.3926
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 C -8.5508 7.3282 2.6347
 C -8.4158 5.9927 1.9116
 C -8.3793 6.1100 0.3896
 N -7.9816 4.9594 -0.2434
 O -8.7237 7.1162 -0.2163
 H -9.9604 -3.3505 4.1108
 H -11.4537 -4.2090 4.5356
 H -11.4688 -2.9831 3.2584
 H -11.4417 -5.3100 2.2542
 H -8.6696 -3.8698 -0.9873
 H -7.5240 5.4511 2.2371
 H -9.2663 5.3440 2.1587
 H -7.4748 4.2506 0.2737
 H -7.8232 5.0252 -1.2381
 H -9.4276 7.8736 2.2777
 H -8.6445 7.1745 3.7138
 H -7.6783 7.9625 2.4533
 H -9.9507 -5.6623 3.1388
 H -9.2906 -2.3303 -0.3630
 H -10.2465 -3.2626 -1.5353
 H -11.1944 -4.3754 0.2467
 O 3.5546 1.2559 -0.4252
 H 3.3263 2.0699 0.0953
 H 4.5270 1.1910 -0.4634

APH⁺

C 11.4811 5.1447 -2.0499
 C 10.3519 4.0984 -2.1775
 C 10.0115 3.3378 -0.9201
 C 8.7717 3.1334 -0.3442
 N 10.9747 2.6596 -0.1929
 C 10.3278 2.0733 0.7983
 N 8.9886 2.3212 0.7564
 H 11.2024 5.9403 -1.3519
 H 10.6453 3.3741 -2.9498
 H 9.4396 4.5825 -2.5462
 H 7.7905 3.5030 -0.5943
 H 10.7723 1.4622 1.5711
 H 8.2970 1.9410 1.4008
 C -9.5797 1.7299 -4.3741
 C -8.5736 2.5669 -3.5651
 C -7.4723 1.7104 -2.9852
 C -6.4371 1.2327 -3.8021
 C -7.4815 1.3081 -1.6449
 C -5.4660 0.3679 -3.3092
 C -6.5131 0.4447 -1.1299
 C -5.5035 -0.0401 -1.9697
 O -4.5387 -0.9061 -1.5627

H	-10.0459	0.9698	-3.7390	C	-0.3705	-1.5311	-1.8506	H	4.7307	-6.8026	-1.9285
H	-9.0958	3.0939	-2.7585	C	-1.6814	-2.0526	-1.3814	H	0.4830	-7.6895	-5.0169
H	-8.1438	3.3380	-4.2166	C	0.3610	-1.9570	-2.9257	H	-1.2838	-7.7824	-5.0196
H	-6.3959	1.5382	-4.8449	C	0.0166	-3.0049	-3.9340	H	3.9804	-5.5205	-6.0260
H	-8.2482	1.6942	-0.9782	C	-0.2520	0.1708	0.0528	H	2.4153	1.1441	4.1494
H	-4.6702	-0.0061	-3.9446	H	2.2012	0.5094	-1.1854	H	-4.5990	1.5425	0.8677
H	-6.5171	0.1927	-0.0765	H	-0.0689	3.5215	-2.0882	C	2.1001	6.5675	-3.9281
H	-4.5277	-1.0773	-0.5846	H	-0.5209	-0.6191	0.7576	C	0.8851	5.9809	-3.2509
C	-0.4311	-7.1573	-4.7376	H	0.5759	0.7417	0.4779	O	0.7658	4.7633	-3.0790
C	-0.4341	-6.8514	-3.2361	H	-5.3340	3.0158	-1.7890	N	-0.0718	6.8655	-2.8629
C	-1.6823	-6.1698	-2.7010	H	-5.4037	3.5954	-0.1166	C	-1.4128	6.3719	-2.6102
C	-1.8870	-6.0836	-1.3163	H	-4.4726	4.5076	-1.3578	C	-2.0182	5.8257	-3.9155
C	-2.6547	-5.5969	-3.5314	H	-2.8011	0.0578	1.1121	O	-1.7456	6.3509	-4.9919
C	-3.0103	-5.4623	-0.7777	H	-1.6764	-2.2218	-0.3015	N	-2.8620	4.7830	-3.7449
C	-3.7879	-4.9733	-3.0096	H	-1.8910	-3.0057	-1.8654	C	-3.4249	4.0631	-4.8794
C	-3.9756	-4.9112	-1.6277	H	-2.4966	-1.3709	-1.6317	C	-2.9674	2.5992	-4.8916
O	-5.1203	-4.3296	-1.1667	H	-0.7598	-3.6657	-3.5461	C	-1.4449	2.3954	-4.8775
H	-0.4749	-6.2419	-5.3367	H	0.8889	-3.6169	-4.1817	C	-1.1121	0.9144	-4.6658
H	-0.2819	-7.7840	-2.6788	C	2.3947	-2.1312	7.2092	C	-0.7642	2.9583	-6.1296
H	0.4395	-6.2261	-3.0015	C	1.6661	-0.7864	7.1782	H	2.9777	5.9724	-3.6732
H	-1.1536	-6.5161	-0.6415	C	2.3468	0.1870	6.2155	H	1.9470	6.5085	-5.0109
H	-2.5404	-5.6407	-4.6093	O	2.4293	-0.2284	4.9839	H	-1.3873	5.6107	-1.8279
H	-3.1391	-5.4059	0.3003	O	2.7708	1.2775	6.6132	H	-2.0271	7.2011	-2.2497
H	-4.5368	-4.5344	-3.6596	C	-7.9451	3.0872	3.9387	H	-3.4019	2.0945	-4.0208
H	-5.0954	-4.2568	-0.2018	C	-7.0765	1.9160	3.4775	H	-3.4014	2.1094	-5.7745
C	4.7574	-4.8222	-5.6916	C	-6.3050	2.1761	2.1828	H	-1.0428	2.9459	-4.0221
C	4.6619	-4.6000	-4.1936	O	-6.4401	3.2671	1.5919	H	0.3153	2.7780	-6.0950
O	5.1158	-3.5990	-3.6429	O	-5.5364	1.2178	1.7996	H	-1.1553	2.4863	-7.0397
C	4.6960	-3.5131	-6.4778	H	-8.4447	2.8494	4.8836	H	-0.9132	4.0384	-6.2098
H	5.7195	-5.3209	-5.8696	H	-7.3423	3.9853	4.0879	H	-1.4832	0.3015	-5.4970
H	5.4389	-2.8126	-6.0916	H	-7.6805	1.0124	3.3237	H	-1.5675	0.5331	-3.7447
H	3.7124	-3.0425	-6.3793	H	-6.3369	1.6456	4.2402	H	-0.0300	0.7625	-4.5963
H	4.8864	-3.6837	-7.5404	C	-0.3782	2.4368	4.9806	H	-3.1137	4.5970	-5.7784
N	4.0805	-5.6206	-3.5028	C	-0.2754	1.8051	3.5840	C	-4.6664	-2.8870	3.7774
C	4.3124	-5.7992	-2.0782	C	0.9901	2.1843	2.8845	C	-3.2493	-2.2799	3.8569
C	3.0819	-5.6328	-1.1900	C	1.2468	2.9114	1.7388	O	-3.0823	-1.0665	3.9558
C	2.5169	-4.2086	-1.1190	N	2.2321	1.8587	3.3900	C	-5.6212	-1.9771	2.9856
C	1.2452	-4.2105	-0.2673	C	3.1633	2.3725	2.5598	C	-5.3663	-1.9985	1.4936
C	3.5505	-3.2118	-0.5796	N	2.6132	3.0200	1.5358	N	-6.3507	-2.4902	0.7143
H	3.7905	-6.4300	-4.0316	H	0.4803	2.1685	5.6021	O	-4.3018	-1.5841	0.9967
H	5.0847	-5.0850	-1.7927	H	-0.3435	0.7150	3.6732	N	-2.1993	-3.1481	3.9042
H	3.3591	-5.9544	-0.1769	H	-1.1240	2.1156	2.9649	C	-0.8421	-2.6690	4.1565
H	2.2966	-6.3229	-1.5274	H	0.5375	3.3928	1.0804	C	-0.1562	-2.1597	2.8787
H	2.2558	-3.9097	-2.1432	H	4.2215	2.2299	2.7150	O	-0.6260	-2.3947	1.7547
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 C 2.4013 0.4521 6.5131
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 H 0.6722 3.3171 0.8364
 H 4.2887 2.0478 2.6104
 H 3.2035 2.9429 0.5240
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Benzoylformate Model D

AP

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C 11.1173 4.0900 -0.9240
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C 8.6116 3.4387 -1.0112
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C 8.5778 2.3359 0.8968
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APH⁺

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YI

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H	9.8074	-4.9440	0.0468	H	5.2289	3.3940	1.2964	C	-0.6639	-2.5460	2.8501
H	7.2825	-4.8062	0.1051	H	5.1209	5.1355	1.0563	O	-1.0406	-2.7178	1.6854
H	7.2357	-5.1620	-1.6228	H	-0.2722	-2.4114	-5.3177	C	-0.6353	-4.6134	4.2422
H	7.0777	-3.3806	-3.1012	H	-8.8633	1.7763	4.1286	C	-1.3165	-5.5100	3.1959
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H	7.2483	-0.9485	-3.6161	H	12.3028	5.7353	-0.8381	N	0.4215	-1.8422	3.2112
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N	-2.2915	3.0907	-0.7339	H	-0.0776	-1.5719	7.3717	O	6.6445	-2.0838	4.9450
C	-3.3941	2.7784	-0.0719	H	1.0326	-1.2002	8.7006	C	6.2966	-1.2769	2.0759
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S	1.5518	-0.6626	-3.5086	H	1.1860	-0.6334	7.9463	N	4.9116	-0.6095	5.0666
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C	-4.5162	3.7642	-0.0101	H	9.0547	-6.4494	-0.5059	H	-6.9963	-2.3897	2.7178
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C	-0.3949	-1.6092	-2.1469	H	4.6320	-6.5672	-2.1238	H	-5.1348	-4.1544	2.9112
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C	0.2615	-1.8445	-3.3145	H	-1.0191	-7.2868	-5.5671	H	0.4464	-4.5304	4.1124
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H	-4.4049	4.3879	0.8843	C	-1.3878	6.4442	-1.6098	H	7.2756	-1.6545	2.3859
H	-4.4837	4.4184	-0.8819	C	-1.9996	6.1851	-2.9983	H	6.1120	-1.6010	1.0454
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C	1.6884	-2.8271	7.4034	C	-0.9082	2.8118	-5.3359	H	0.0174	7.9939	-1.8647
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C	-8.4021	2.7562	3.9612	C	4.8931	0.9417	-4.4652	H	-7.2596	-3.0240	0.5357
C	-6.9022	2.6065	3.6835	C	4.6761	1.0441	-3.0923	H	-6.1365	-2.4882	-0.6980
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H	-8.5894	3.3699	4.8480	O	5.3136	1.1369	-0.0883	C	-9.8578	-4.3240	0.7221
H	-8.9007	3.2090	3.1053	O	3.2739	0.3363	0.4583	O	-8.7547	-3.9129	1.0945
H	-6.4196	1.9481	4.4104	H	3.0275	6.3885	-2.4251	C	-11.2732	-4.1537	2.7499
H	-6.4119	3.5859	3.7844	H	2.2107	6.9909	-3.8718	N	-10.3663	-4.0480	-0.4989
C	-0.9271	1.9602	5.4632	H	-1.3578	5.5343	-1.0076	C	-9.6658	-3.2055	-1.4525
C	-0.8725	1.3880	4.0434	H	-2.0039	7.1775	-1.0827	C	-8.9572	7.0087	3.1276
C	0.3815	1.7743	3.3277	H	-3.9873	2.6848	-3.6892	C	-8.6496	5.7965	2.2596
C	0.5449	2.5191	2.1864	H	-3.7241	2.7888	-5.4161	C	-8.2570	6.1500	0.8250
N	1.6369	1.3860	3.7825	H	-1.5176	2.7096	-3.3099	N	-7.7537	5.0973	0.1286
C	2.5200	1.8738	2.9198	H	0.0402	2.2865	-5.1819	O	-8.4066	7.2729	0.3508
N	1.9022	2.5795	1.9460	H	-1.2676	2.5746	-6.3454	H	-10.4323	-3.6891	3.3268
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C	5.8503	4.5467	3.0403	H	5.5970	0.2085	-4.8449	H	-9.7340	7.6243	2.6677
C	5.8332	3.2989	3.9358	H	5.2145	0.4012	-2.4056	H	-9.2923	6.6982	4.1221
C	4.9841	4.3370	1.7916	C	-5.1106	-3.1887	3.4220	H	-8.0729	7.6420	3.2447
H	4.6641	7.0944	2.2677	C	-3.6838	-2.7077	3.6924	H	-10.1545	-5.8985	2.1107
H	4.3958	5.5818	4.2463	O	-3.4477	-1.5368	3.9814	H	-9.3892	-2.2527	-0.9924
H	6.0574	5.8749	4.7270	C	-5.9339	-2.1422	2.6439	H	-10.3190	-3.0115	-2.3037
H	6.8857	4.7099	2.7069	C	-5.5348	-2.0533	1.1853	H	-11.2711	-4.4178	-0.7419
H	4.8277	3.1299	4.3406	N	-6.3409	-2.6602	0.2810				
H	6.1330	2.3961	3.3941	O	-4.4969	-1.4730	0.8290				

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TCH⁺

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C	8.0394	-2.3942	-0.7755	H	4.9806	3.0443	4.3436	N	-6.3849	-3.1301	0.2919
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C	8.0689	-0.6520	-2.4456	H	4.1372	4.2451	2.0525	C	-1.2901	-3.1360	4.2628
H	9.6522	-4.7797	-0.0571	H	5.4981	3.3789	1.3168	C	-0.5296	-2.7524	2.9879
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N	-0.4024	1.8828	-0.9853	H	5.2081	7.8689	3.8608	C	5.6883	-1.7299	4.4365
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S	1.2386	0.3199	-2.5405	H	1.2962	-3.8148	7.7534	N	4.9900	-0.7463	5.0492
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C	-4.6132	4.0188	-0.3471	H	9.2379	-6.4072	-0.6245	H	-6.9460	-2.5818	2.7035
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C	-0.6645	-1.2024	-1.6149	H	4.6555	-6.5217	-2.3236	H	-4.9597	-4.2256	2.8768
C	-1.7641	-2.1836	-1.3840	H	0.7854	-6.5207	-5.8189	H	-0.8547	-4.4287	5.9528
C	-0.0126	-0.9452	-2.7643	H	-0.4147	-7.4320	-4.8841	H	0.4552	-4.3676	4.7532
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H	1.3480	0.9499	-0.2112	H	-5.0629	1.8319	1.2371	H	-3.4006	-5.3903	4.7826
H	-0.1207	2.6834	-1.5450	C	2.2695	7.0431	-2.6620	H	-3.1977	-5.4070	3.0193
H	-1.4807	-1.2229	0.9616	C	1.1027	6.1838	-2.2030	H	-1.3220	-2.2842	4.9474
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H	-5.5617	3.8703	0.1721	C	-1.1767	6.2135	-1.3986	H	7.3208	-1.8226	2.3659
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H	-0.9375	-2.3284	-4.1026	C	-2.4052	2.2509	-4.1092	H	-4.0657	5.3431	-4.4352
H	0.8052	-2.1317	-4.3588	C	-2.9092	0.8144	-4.2554	H	-2.5384	4.2698	-2.2795
C	1.8242	-2.9661	7.3085	C	-1.1606	2.5151	-4.9627	H	0.0970	7.8489	-1.6568
C	1.0682	-1.6562	7.5745	C	4.1167	2.0857	-2.5358	H	5.9736	-0.8860	6.8645
C	1.6714	-0.4747	6.8377	C	3.4964	2.9775	-3.4273	H	4.6452	0.3091	6.8150
O	1.5235	-0.5904	5.5124	C	3.7921	2.9068	-4.7844	H	4.2768	-0.2845	4.5068
O	2.2102	0.4734	7.3766	C	4.7014	1.9556	-5.2574	H	0.6385	-1.5845	4.1739
C	-8.2771	2.6950	4.0281	C	5.3189	1.0695	-4.3716	H	-7.2446	-3.5648	0.6212
C	-8.4352	1.8873	2.7283	C	5.0266	1.1279	-3.0123	H	-6.1898	-3.1615	-0.7046
C	-7.2485	2.1190	1.7932	C	3.7328	2.1318	-1.1103	H	3.9056	-0.8325	1.8869
O	-7.3290	3.0196	0.9205	O	2.9778	3.0026	-0.6655	H	-5.4223	-3.3920	4.3450
O	-6.2151	1.3999	1.9979	C	4.2800	1.0737	-0.1454	C	-11.0678	-5.0585	1.4227
H	-9.0899	2.4732	4.7274	O	5.5372	1.0984	0.0003	C	-10.0077	-4.4764	0.5099
H	-7.3298	2.4447	4.5150	O	3.4540	0.3475	0.4430	O	-8.8145	-4.5153	0.8249
H	-9.3547	2.1793	2.2121	H	3.1909	6.4631	-2.5873	C	-11.1566	-4.1864	2.6796
H	-8.4879	0.8201	2.9663	H	2.1115	7.3050	-3.7132	N	-10.4539	-3.8657	-0.6095
C	-0.7966	1.8630	5.4827	H	-1.0648	5.2315	-0.9375	C	-9.5656	-3.1483	-1.5077
C	-0.7500	1.4096	4.0221	H	-1.8063	6.8262	-0.7465	C	-8.8334	6.9642	3.2890
C	0.5257	1.7874	3.3391	H	-4.3854	3.0133	-3.7187	H	-10.1773	-4.1269	3.1599
C	0.7171	2.5411	2.2074	H	-3.9317	3.0665	-5.4107	H	-11.8717	-4.5990	3.3968
N	1.7660	1.3531	3.7943	H	-2.1096	2.3737	-3.0627	H	-11.4748	-3.1693	2.4298
C	2.6676	1.8227	2.9419	H	-0.3869	1.7725	-4.7466	H	-12.0405	-5.1258	0.9226
N	2.0766	2.5599	1.9745	H	-1.3977	2.4639	-6.0332	H	-8.7555	-3.8016	-1.8436
H	0.0685	1.5088	6.0442	H	-0.7271	3.4980	-4.7531	H	-8.4090	6.8968	4.2958
H	-0.8881	0.3239	3.9640	H	-3.1578	0.5859	-5.2996	H	-8.9286	8.0159	3.0111
H	-1.5872	1.8452	3.4664	H	-3.8115	0.6549	-3.6619	H	-9.8406	6.5345	3.3176
H	0.0229	3.0572	1.5653	H	-2.1564	0.1020	-3.9138	H	-10.7571	-6.0731	1.6882
H	3.7282	1.6280	2.9700	H	-2.4562	5.0067	-5.0514	H	-9.1157	-2.2775	-1.0201
H	2.5144	2.8661	1.0975	H	2.7697	3.6901	-3.0477	H	-10.1321	-2.8132	-2.3768
C	5.5138	7.0572	3.1923	H	3.3045	3.5858	-5.4773	H	-11.4466	-3.8372	-0.7791
C	5.5135	5.7114	3.9255	H	4.9263	1.9029	-6.3190	C	-7.9607	6.2446	2.2669
C	6.0191	4.5068	3.1082	H	6.0264	0.3312	-4.7337	C	-8.4789	6.4980	0.8483
C	5.9960	3.2412	3.9779	H	5.5089	0.4434	-2.3249	N	-8.5553	5.3965	0.0619
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H -6.9393 6.6444 2.3065
H -7.8862 5.1724 2.4565
H -8.2334 4.4782 0.3752
H -8.8439 5.5361 -0.8945

**R-Mandelate
Model E**

AP

C 11.1550 5.6121 0.0247
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C	4.5043	-3.0980	-5.0809	H	-9.1193	2.8470	4.4198	O	5.6391	1.2238	-0.2895
H	6.2678	-4.2671	-5.5282	H	-7.4022	2.4177	4.2843	O	3.5250	0.7264	0.2823
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H	3.1785	-1.9671	-0.3791	C	5.2822	4.5006	1.4751	C	-4.8715	-2.9917	3.6232
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C	7.9190	-2.4871	-0.7611	H	4.8494	3.4596	4.0833	N	-6.2865	-3.2635	0.6073
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