Evaluating Theoretical Solvent Models for Thermodynamic and Structural Descriptions of Dacarbazine–Cyclodextrin Complexes. The Theoretical and Conductometric Study

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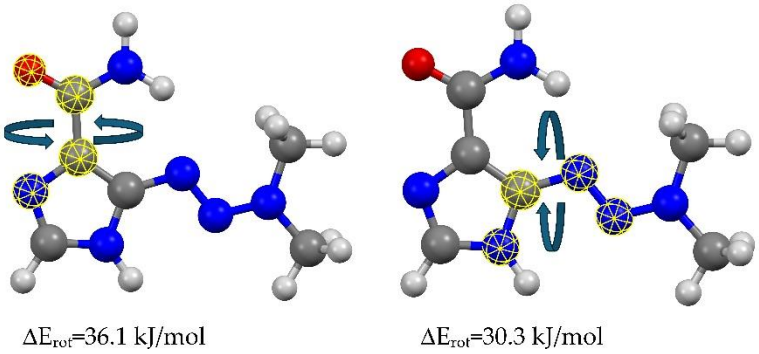


Figure S1. Schematic representation of torsion angles (highlighted in yellow) scanned from 0° to 360° in 10° increments to compute the rotational energy profile and determine the barrier (ΔE$_{rot}$) for the carboxamide and 3,3-dimethyltriaz-1-en-1-yl groups.

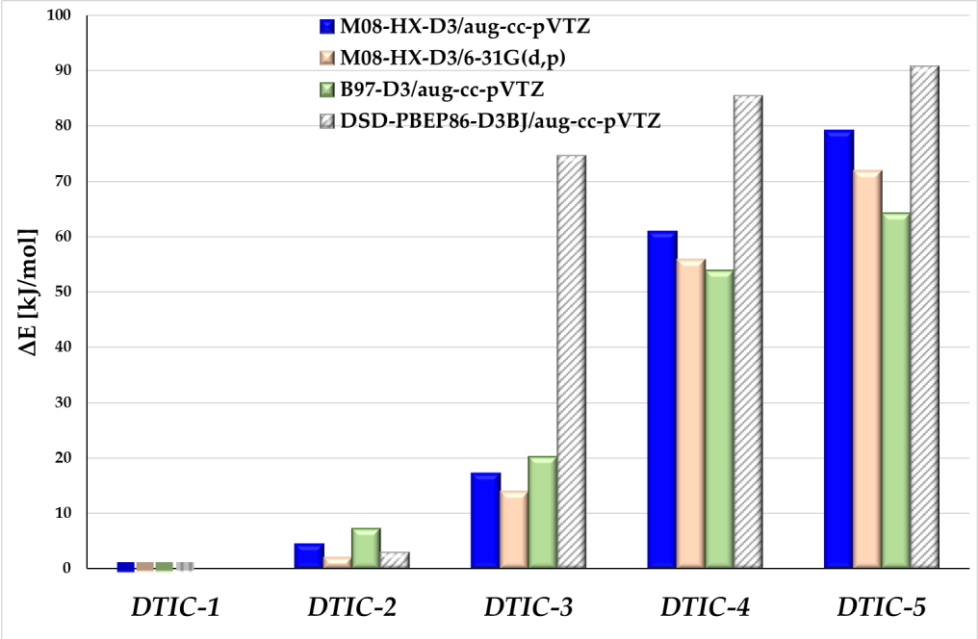


Figure S2. The relative energy differences (ΔE, in kJ/mol) between DTIC-1 and four other, less stable conformers obtained at the M08-HX-D3/aug-cc-pVTZ, M08-HX-D3/6-31G(d,p), B97-D3/aug-cc-pVTZ, and DSD-PBEP86-D3BJ/aug-cc-pVTZ theory levels.

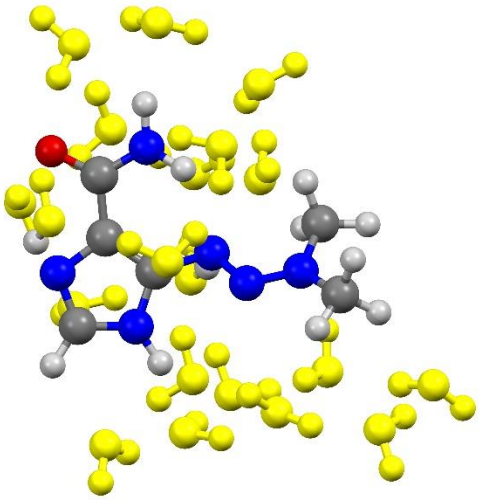


Figure S3. DTIC-1 in the presence of twenty water molecules (highlighted in yellow; DTIC-1 (20 H_2O)). The structure was optimized at the M08-HX-D3/aug-cc-pVTZ theory level.

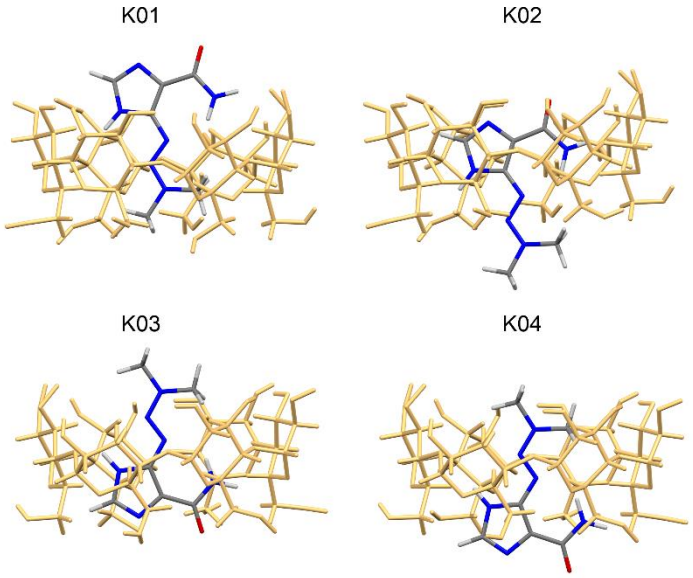


Figure S4. Initial models of complex CDs:DTIC. Cyclodextrin is highlighted in dark yellow.

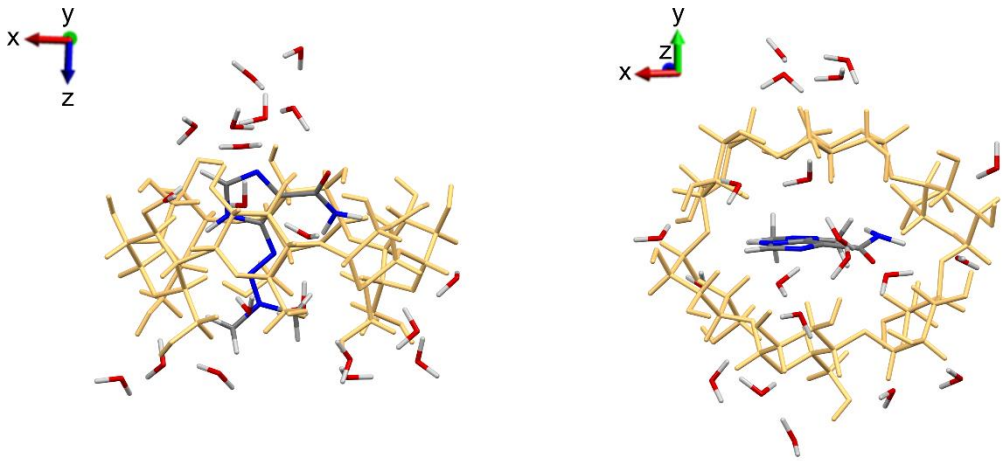


Figure S5. The most stable *α*-CD:DTIC complex, K02_03, obtained from calculations performed at the M08-HX-D3/6-31G(d,p) theory level in the presence of twenty explicitly added water molecules. Cyclodextrin is highlighted in dark yellow.

Table S1. Total energy values [Hartree] obtained at the M08-HX-D3/6-31G(d,p) theory level in water (PCM) for the most stable complexes presented in Figure 4 of the main article.

Molecule	**Energy**
α-CD:DTIC K02_03	-4301.6460
α-CD:DTIC K01_01	-4301.6394
α-CD:DTIC K03_03	-4301.6382
HP-β-CD:DTIC K03_03	-5684.6240
HP-β-CD:DTIC K04_03	-5684.6202
HP-β-CD:DTIC K04_01	-5684.6175
HE-β-CD:DTIC K04_01	-5527.3902
HE-β-CD:DTIC K03_02	-5527.3794
HE-β-CD:DTIC K03_03	-5527.3792

Table S2. Coordinates [Å] of the most stable complexes, presented in Figure 4 of the main article, obtained at the M08-HX-D3/6-31G(d,p) theory level in water (PCM).

***α*-CD:DTIC**									
Atomic Number	**K02_03**			**K01_01**			**K03_03**		
	x	**y**	**z**	**x**	**y**	**z**	**x**	**y**	**z**
6	-5.6569	0.1832	0.2741	-5.0105	-2.3067	0.7305	0.3650	-4.5145	-1.1463
6	-5.9616	1.1842	-0.8356	-5.8512	-1.7150	-0.3973	-0.5302	-4.0515	-2.2901
6	-4.7543	2.0889	-1.0402	-5.3208	-0.3262	-0.7216	-1.4493	-2.9600	-1.7562
6	-4.1849	2.6678	0.2579	-5.1809	0.5587	0.5195	-2.2629	-3.5105	-0.5901
6	-4.2098	1.6682	1.4237	-4.6225	-0.2117	1.7217	-1.3255	-4.0932	0.4811
6	-4.1424	2.3622	2.7752	-4.8081	0.4997	3.0465	-2.0434	-4.8864	1.5766
6	-2.6350	-4.1621	-0.1856	-0.3021	-4.6348	0.1234	5.0499	-2.2920	-0.4357
6	-3.6397	-3.9468	-1.3213	-1.3079	-4.7782	-1.0211	4.7483	-3.3147	-1.5323
6	-4.0356	-2.4808	-1.3650	-2.2007	-3.5463	-1.0234	3.2459	-3.3383	-1.7859
6	-4.4844	-1.9752	-0.0003	-2.8933	-3.4567	0.3263	2.4833	-3.6055	-0.4913
6	-3.4873	-2.3528	1.0978	-1.8280	-3.3725	1.4251	2.9050	-2.5989	0.5736
6	-4.0490	-2.1074	2.4887	-2.4429	-3.3505	2.8118	2.3514	-2.8968	1.9557

6	2.6106	-4.1184	-0.5312	4.4366	-2.5505	-0.7120	4.2818	2.7446	0.4816
6	1.9073	-3.9729	-1.8904	3.5859	-2.7461	-1.9736	5.1718	2.5905	-0.7523
6	0.4985	-3.4010	-1.7384	2.1024	-2.6458	-1.6068	4.9440	1.2083	-1.3226
6	-0.2531	-4.1130	-0.6223	1.8079	-3.6286	-0.4851	5.2270	0.1245	-0.2907
6	0.5583	-4.0882	0.6697	2.6938	-3.3303	0.7229	4.5954	0.4154	1.0863
6	-0.1129	-4.8423	1.8036	2.4888	-4.3600	1.8235	5.3598	-0.2336	2.2417
6	5.8417	-0.2310	0.6619	4.8879	2.1482	0.6653	-0.4266	4.7313	-0.6716
6	6.2839	-1.1907	-0.4490	5.6884	1.5805	-0.5525	0.4085	4.3424	-1.8981
6	5.0815	-2.0439	-0.8622	6.2601	0.1880	-0.2472	1.3784	3.2277	-1.5049
6	4.2801	-2.5805	0.3359	5.2790	-0.6997	0.5219	2.1725	3.6350	-0.2707
6	4.1618	-1.6393	1.5400	4.5900	0.0602	1.6743	1.2357	4.0630	0.8591
6	3.8743	-2.4083	2.8342	4.7795	-0.6392	3.0126	1.9884	4.6036	2.0642
6	2.7567	4.1134	0.2539	0.2366	4.6728	0.5010	-5.1285	2.4448	-0.0796
6	3.8355	4.0297	-0.8309	1.1972	4.8934	-0.6773	-4.8585	3.5721	-1.0798
6	4.3203	2.5881	-0.9577	2.0794	3.6585	-0.8087	-3.3563	3.6471	-1.3575
6	4.6905	1.9493	0.3726	2.7926	3.3743	0.4981	-2.5597	3.7822	-0.0658
6	3.5582	2.1700	1.3816	1.7579	3.2205	1.6113	-2.9631	2.6524	0.8785
6	3.9171	1.7869	2.8094	2.3796	3.0595	2.9857	-2.3075	2.7462	2.2374
6	-2.4630	4.2823	-0.3349	-4.5467	2.7672	-0.3227	-4.3805	-2.6931	0.2015
6	-1.6982	4.2415	-1.6641	-3.7553	2.9286	-1.6272	-5.2428	-2.3916	-1.0228
6	-0.3689	3.5186	-1.4873	-2.2585	2.8624	-1.3180	-5.0197	-0.9458	-1.4318
6	0.4249	4.1663	-0.3661	-1.9211	3.8518	-0.2078	-5.3283	0.0185	-0.2906
6	-0.4339	4.1569	0.9057	-2.8665	3.7496	0.9948	-4.6835	-0.4403	1.0354
6	0.2231	4.8700	2.0744	-2.6706	4.8914	1.9784	-5.3766	0.0976	2.2880
1	-6.5063	-0.4876	0.4702	-5.3170	-3.3302	0.9956	1.0358	-5.3275	-1.4627
1	-6.8360	1.7837	-0.5288	-6.9013	-1.6560	-0.0629	-1.1297	-4.9111	-2.6402
1	-3.9598	1.4615	-1.4655	-4.3011	-0.4549	-1.1270	-0.8085	-2.1491	-1.3689
1	-4.3103	3.3587	-2.4258	-5.6317	0.8717	-2.1956	-3.1234	-2.8199	-2.7447
1	-4.7559	3.5764	0.5245	-6.1553	1.0253	0.7544	-2.9346	-4.3093	-0.9577
1	-3.3364	0.9948	1.3263	-3.5441	-0.3242	1.5503	-0.7643	-3.2540	0.9366
1	-3.1879	2.9008	2.8569	-4.3921	1.5143	2.9685	-2.7651	-5.5760	1.1096
1	-5.0490	0.9548	3.7230	-4.4979	-1.0592	4.1326	-2.0745	-3.7207	3.1134
1	-4.9616	3.0995	2.8470	-5.8840	0.5846	3.2806	-1.2823	-5.5047	2.0808
1	-2.3794	-5.2266	-0.0652	0.3578	-5.5136	0.2056	6.1146	-2.3016	-0.1474
1	-4.5290	-4.5719	-1.1281	-1.9218	-5.6794	-0.8491	5.0623	-4.3053	-1.1509
1	-3.5874	-4.0424	-3.2511	-1.2376	-4.8827	-2.9522	5.0292	-3.4804	-3.4127
1	-3.1199	-1.9271	-1.6446	-1.5560	-2.6496	-1.1168	2.9504	-2.3393	-2.1493
1	-5.2983	-1.3714	-2.3384	-3.9069	-3.1410	-1.8954	2.1594	-4.0726	-3.2173
1	-5.4828	-2.3725	0.2482	-3.5308	-4.3413	0.4986	2.6762	-4.6310	-0.1270
1	-2.5549	-1.7766	0.9612	-1.2139	-2.4672	1.2752	2.5669	-1.5973	0.2522
1	-3.2767	-2.3630	3.2352	-1.6355	-3.3467	3.5636	2.6227	-2.0594	2.6303
1	-5.0132	-3.7726	2.5302	-2.8244	-5.2415	2.8677	3.7935	-4.1009	2.3588
1	-4.2972	-1.0403	2.6015	-3.0230	-2.4219	2.9277	1.2544	-2.9518	1.9222
1	3.5180	-4.7325	-0.6384	5.4964	-2.7671	-0.9241	4.3968	3.7458	0.9311
1	1.8312	-4.9636	-2.3612	3.7876	-3.7462	-2.3880	6.2207	2.7058	-0.4266
1	2.6183	-2.2536	-2.4207	4.0482	-0.9488	-2.4875	5.3807	3.4092	-2.4875

1	0.5873	-2.3361	-1.4287	1.9184	-1.6364	-1.2125	3.8765	1.1466	-1.6059
1	-1.1334	-3.5332	-2.7742	0.7659	-3.6729	-2.6025	5.5950	0.1790	-2.8168
1	-0.4462	-5.1597	-0.9165	1.9913	-4.6631	-0.8312	6.3206	0.0120	-0.1719
1	0.7397	-3.0383	0.9626	2.4540	-2.3155	1.0890	3.5410	0.0868	1.0573
1	0.5375	-4.7937	2.6942	3.1309	-4.1157	2.6856	4.7979	-0.0466	3.1747
1	0.4385	-6.5778	1.1603	3.6255	-5.6739	0.9820	6.5761	1.2468	2.3660
1	-1.0692	-4.3595	2.0474	1.4430	-4.3206	2.1599	5.4324	-1.3165	2.1039
1	6.6773	0.3968	1.0063	5.2298	3.1623	0.9178	-1.0804	5.5906	-0.8879
1	7.0863	-1.8366	-0.0623	6.5446	2.2550	-0.7316	0.9853	5.2309	-2.2196
1	6.2147	0.3052	-1.6797	4.3987	2.3144	-1.8221	-1.2734	4.3107	-2.8849
1	4.4166	-1.3813	-1.4348	6.4773	-0.3012	-1.2156	0.7677	2.3526	-1.2279
1	4.7409	-3.3128	-2.2751	8.0962	0.7426	0.0950	3.0887	3.2348	-2.4340
1	4.7600	-3.5257	0.6551	5.8721	-1.5433	0.9202	2.8529	4.4694	-0.5131
1	3.3395	-0.9248	1.3349	3.5128	0.0987	1.4296	0.6271	3.1859	1.1506
1	4.7678	-3.0102	3.0770	5.8559	-0.6906	3.2530	1.2571	4.9179	2.8272
1	2.8096	-3.8940	2.1064	4.6091	-2.4629	2.3162	2.3080	6.3233	1.2519
1	3.7310	-1.6858	3.6520	4.2817	-0.0604	3.8038	2.6132	3.8120	2.5057
1	2.4911	5.1582	0.4795	-0.3684	5.5747	0.6896	-6.1838	2.4191	0.2390
1	4.6736	4.6881	-0.5580	1.8203	5.7770	-0.4675	-5.1950	4.5221	-0.6389
1	2.4959	3.9978	-2.2303	-0.0785	4.3799	-2.0661	-5.4575	2.4606	-2.5261
1	3.4609	2.0312	-1.3680	1.4071	2.8072	-1.0287	-3.0480	2.6996	-1.8414
1	5.1702	2.8274	-2.6733	2.6053	4.0990	-2.6184	-3.7031	4.7122	-2.9299
1	5.6443	2.3610	0.7484	3.4792	4.2083	0.7328	-2.7518	4.7673	0.3991
1	2.6701	1.5982	1.0434	1.1213	2.3432	1.3859	-2.6482	1.6975	0.4193
1	4.8219	2.3465	3.1090	3.0073	3.9435	3.2031	-2.6884	3.6314	2.7742
1	2.6424	2.9883	3.6014	0.7419	3.5880	3.8438	-2.2040	1.5672	3.7932
1	4.1523	0.7159	2.8711	3.0309	2.1723	2.9895	-1.2197	2.8535	2.0961
1	-1.8692	3.2620	-3.3185	-3.4199	1.4871	-2.9566	-5.4105	-2.9516	-2.8516
1	-3.3615	4.9139	-0.4216	-5.6315	2.8196	-0.5092	-4.5173	-3.7279	0.5544
1	-1.4999	5.2847	-1.9712	-3.9781	3.9292	-2.0390	-6.2992	-2.5482	-0.7414
1	-0.5923	2.4799	-1.1901	-1.9956	1.8407	-0.9784	-3.9506	-0.8427	-1.6909
1	0.7310	2.6946	-2.9032	-1.4405	2.4715	-3.0545	-5.3355	-0.1898	-3.2060
1	0.6677	5.2100	-0.6357	-1.9854	4.8716	-0.6294	-6.4220	0.1090	-0.1612
1	-0.6622	3.1108	1.1807	-2.6901	2.7927	1.5136	-3.6208	-0.1450	1.0011
1	1.1433	4.3389	2.3530	-1.6651	4.8259	2.4188	-5.3825	1.1901	2.3047
1	-0.2217	6.6255	1.4113	-3.6390	6.1714	0.9078	-6.6727	-1.3200	2.2604
1	-0.4641	4.8472	2.9365	-3.4049	4.7819	2.7938	-4.7949	-0.2483	3.1615
8	-6.2250	0.4654	-2.0251	-5.7301	-2.5421	-1.5402	0.2879	-3.5533	-3.3307
8	-5.1210	3.0891	-1.9649	-6.1716	0.2339	-1.6991	-2.2376	-2.4239	-2.7973
8	-2.8088	2.9818	0.0562	-4.1908	1.5487	0.2676	-3.0209	-2.4334	-0.0543
8	-5.4086	0.8931	1.4593	-5.1929	-1.5103	1.8747	-0.4292	-5.0342	-0.1111
8	-4.2091	1.4198	3.8244	-4.1037	-0.1807	4.0667	-2.7413	-4.0751	2.4943
8	-3.0057	-4.3184	-2.5304	-0.5888	-4.8986	-2.2355	5.4447	-2.9701	-2.7043
8	-5.0414	-2.3097	-2.3360	-3.0911	-3.6288	-2.1129	2.9933	-4.3108	-2.7818
8	-4.5297	-0.5531	-0.1302	-3.6720	-2.2763	0.3038	1.0986	-3.4009	-0.7141
8	-3.2061	-3.7526	1.0327	-0.9868	-4.5292	1.3464	4.3273	-2.6399	0.7252

8	-5.2344	-2.8466	2.6913	-3.3332	-4.4319	3.0001	2.8317	-4.1346	2.4373
8	2.7134	-3.1681	-2.7346	3.9789	-1.8022	-2.9422	4.8364	3.5827	-1.7069
8	-0.1798	-3.5148	-2.9630	1.2693	-2.8502	-2.7324	5.7734	1.0568	-2.4544
8	-1.4788	-3.4073	-0.4654	0.4532	-3.4662	-0.1018	4.6768	-1.0351	-0.9126
8	1.8072	-4.7592	0.4320	4.0766	-3.4063	0.3487	4.6614	1.8125	1.4460
8	-0.3976	-6.1757	1.4274	2.7299	-5.6689	1.3429	6.6695	0.2874	2.3094
8	6.8018	-0.4556	-1.5323	4.8936	1.4813	-1.7139	-0.4169	3.8563	-2.9308
8	5.4860	-3.1167	-1.6866	7.4034	0.2749	0.5746	2.2093	2.8526	-2.5805
8	2.9383	-2.8281	-0.0881	4.2711	-1.2005	-0.3513	2.9202	2.5022	0.1759
8	5.3702	-0.9319	1.7817	5.0943	1.3805	1.8173	0.3925	5.1189	0.4063
8	2.7079	-3.1979	2.7697	4.1770	-1.9180	2.9886	2.8513	5.6604	1.6971
8	3.3303	4.4724	-2.0722	0.5095	5.1376	-1.8798	-5.5619	3.3925	-2.2883
8	5.4350	2.4654	-1.8181	3.0592	3.7963	-1.8206	-3.0619	4.7443	-2.2055
8	4.8345	0.5608	0.0746	3.5226	2.1686	0.3300	-1.1822	3.6022	-0.3247
8	3.2320	3.5592	1.4535	0.9499	4.4008	1.6798	-4.3714	2.6668	1.0832
8	2.8367	2.0463	3.6792	1.3831	2.8767	3.9678	-2.6258	1.5511	2.9269
8	-2.4783	3.5755	-2.6343	-4.1761	1.9320	-2.5376	-4.8850	-3.2475	-2.0941
8	0.3156	3.5579	-2.7243	-1.4789	3.2294	-2.4439	-5.8381	-0.6966	-2.5619
8	1.6207	3.4114	-0.2116	-0.5931	3.5695	0.2060	-4.7796	1.2585	-0.7411
8	-1.6465	4.8770	0.6459	-4.2236	3.8220	0.5542	-4.7935	-1.8604	1.2418
8	0.5817	6.1932	1.7280	-2.7785	6.1508	1.3457	-6.7137	-0.3579	2.3300
1	-6.2076	1.1109	-2.7448	-6.0623	-2.0184	-2.2833	-0.2937	-3.1086	-3.9619
6	-1.9651	0.4443	-2.4213	2.3977	0.9416	-3.2375	1.9552	0.5306	3.7810
7	-0.7794	0.5813	-2.9581	1.2950	0.7625	-3.9346	1.0967	-0.3491	4.2417
6	0.1019	0.3029	-1.9435	0.3515	0.4101	-3.0082	0.1615	-0.5030	3.2467
6	-0.5782	0.0200	-0.7662	0.8923	0.3935	-1.7401	0.4870	0.2928	2.1610
7	-1.8959	0.1237	-1.0954	2.2080	0.7233	-1.9092	1.6347	0.9421	2.5206
6	1.5445	0.5181	-2.0912	-1.0456	0.0015	-3.3380	-0.8808	-1.5626	3.2395
8	1.9999	1.3134	-2.9208	-1.9026	0.8234	-3.7116	-0.6710	-2.6883	3.7202
7	2.3253	-0.2131	-1.2626	-1.2714	-1.2981	-3.1762	-2.0132	-1.2266	2.6119
7	-0.0385	-0.2376	0.4842	0.2063	0.1943	-0.5535	-0.1263	0.4037	0.9038
7	-0.8981	-0.1063	1.4184	0.9363	-0.0864	0.4448	0.7148	0.0917	-0.0002
7	-0.4572	-0.3207	2.6130	0.2541	-0.2325	1.5559	0.2561	0.0522	-1.2104
6	-1.3582	-0.0649	3.7191	0.9922	-0.3502	2.8003	1.2113	-0.2592	-2.2558
6	0.9359	-0.6203	2.8755	-1.1395	0.1589	1.5832	-1.1202	0.3805	-1.5321
1	-2.9114	0.5437	-2.9444	3.3649	1.2234	-3.6418	2.8127	0.9267	4.3154
1	-2.6933	-0.0044	-0.4752	2.9014	0.8604	-1.1723	2.1728	1.5534	1.9052
1	1.8875	-0.7020	-0.4854	-0.4823	-1.8988	-2.9375	-2.1501	-0.2612	2.3312
1	3.2833	0.0850	-1.1160	-2.1911	-1.7067	-3.2996	-2.6947	-1.9359	2.3546
1	-1.4350	-0.9571	4.3543	1.0945	0.6291	3.2974	0.9376	-1.2057	-2.7482
1	-0.9788	0.7680	4.3272	0.4498	-1.0295	3.4693	1.2563	0.5596	-2.9868
1	-2.3463	0.2035	3.3330	1.9800	-0.7817	2.6019	2.1950	-0.3613	-1.7802
1	1.0266	-0.9030	3.9285	-1.5457	-0.0356	2.5836	-1.2584	1.4746	-1.5080
1	1.2762	-1.4531	2.2489	-1.2301	1.2309	1.3294	-1.3414	-0.0133	-2.5300
1	1.5579	0.2700	2.6857	-1.7032	-0.4019	0.8237	-1.7911	-0.0934	-0.7968
HP-β-CD:DTIC									

Atomic Number	K03_03			K04_03			K04_01		
	x	y	z	x	y	z	x	y	z
6	0.9135	-4.8971	-0.4853	4.6357	-3.7648	-0.9372	-1.4455	-4.8840	0.0601
6	0.2972	-5.0733	-1.8940	4.1218	-4.1529	-2.3283	-2.3704	-5.4199	-1.0416
8	1.2194	-4.5895	-2.8658	4.5294	-3.1692	-3.2607	-1.5865	-5.9941	-2.0644
6	-1.0456	-4.3708	-2.0484	2.6032	-4.2629	-2.3382	-3.2731	-4.3272	-1.5916
8	-1.6536	-4.8188	-3.2312	2.2322	-4.7718	-3.5962	-4.1434	-4.9378	-2.5153
6	-1.9234	-4.5856	-0.8185	2.0888	-5.1210	-1.1918	-3.9955	-3.7006	-0.4105
8	-3.1026	-3.8536	-1.0891	0.6756	-4.9524	-1.2136	-4.8960	-2.6990	-0.8518
6	-1.1239	-4.0510	0.3711	2.7042	-4.6178	0.1153	-2.9531	-3.1108	0.5368
8	-0.0333	-4.9599	0.5415	4.1218	-4.7015	-0.0086	-2.1965	-4.2112	1.0502
6	-1.8543	-3.9209	1.6988	2.2874	-5.3810	1.3697	-3.5939	-2.3497	1.6988
8	-1.2273	-2.9791	2.5452	1.0245	-4.9300	1.8278	-3.6856	-0.9517	1.4401
6	-4.3627	-4.4229	-0.8601	-0.1649	-6.0584	-1.0520	-6.2322	-3.1305	-1.0404
6	-5.2176	-4.0856	-2.0850	-1.0941	-6.1482	-2.2654	-6.7586	-2.4804	-2.3061
8	-4.6043	-4.6519	-3.2267	-0.2837	-6.2173	-3.4223	-6.0888	-3.0533	-3.4141
6	-5.2746	-2.5745	-2.2023	-2.0235	-4.9441	-2.3181	-6.4879	-0.9886	-2.2228
8	-6.1360	-2.2219	-3.2595	-2.9445	-5.1576	-3.3605	-7.3087	-0.3566	-3.1804
6	-5.7139	-1.9288	-0.8937	-2.7225	-4.7772	-0.9792	-6.6533	-0.3904	-0.8061
8	-5.4581	-0.5435	-1.0912	-3.4918	-3.5954	-1.0753	-5.4831	0.3938	-0.5153
6	-4.9031	-2.4510	0.2903	-1.6839	-4.6826	0.1341	-6.8558	-1.3715	0.3817
8	-4.9663	-3.8819	0.2941	-0.9349	-5.9133	0.1297	-7.0412	-2.7379	0.0301
6	-5.3083	-1.9126	1.6476	-2.2970	-4.4500	1.4998	-8.0660	-0.9678	1.2229
8	-6.7092	-1.8034	1.7995	-3.4676	-5.2125	1.6530	-7.9670	0.3785	1.6328
6	-7.0572	-1.5401	3.1523	-4.1028	-4.9218	2.8813	-6.9718	0.6145	2.6191
6	-8.3207	-0.6951	3.1837	-5.5145	-5.4868	2.8764	-7.0960	2.0791	3.0353
6	-8.7683	-0.4140	4.6069	-6.1793	-5.2740	4.2331	-8.3606	2.3426	3.8383
8	-8.0706	0.5489	2.5440	-6.2871	-4.9097	1.8342	-5.9274	2.4915	3.7346
6	-6.5035	0.3520	-0.8660	-4.7805	-3.6175	-0.5242	-5.7151	1.7686	-0.2811
6	-6.4202	1.4438	-1.9288	-5.7493	-3.1230	-1.6000	-5.3295	2.6228	-1.5008
8	-6.4463	0.8068	-3.1905	-5.5659	-3.9269	-2.7503	-5.7912	1.9816	-2.6769
6	-5.1544	2.2656	-1.7336	-5.4964	-1.6569	-1.9031	-3.8331	2.8953	-1.6044
8	-5.1948	3.3504	-2.6315	-6.5034	-1.2191	-2.7843	-3.6436	3.8158	-2.6508
6	-5.0410	2.7395	-0.2904	-5.5067	-0.8731	-0.6008	-3.3311	3.3865	-0.2608
8	-3.7578	3.3334	-0.1988	-5.2533	0.4803	-0.9362	-1.9510	3.6912	-0.3757
6	-5.1683	1.5670	0.6799	-4.4643	-1.4370	0.3621	-3.6128	2.2842	0.7566
8	-6.4142	0.9122	0.4173	-4.8457	-2.7960	0.6246	-5.0341	2.1800	0.8644
6	-5.1944	1.9772	2.1459	-4.3835	-0.6647	1.6730	-3.0887	2.5938	2.1485
8	-6.2768	2.8329	2.4346	-5.6548	-0.3370	2.1941	-3.6586	3.7780	2.6549
6	-3.6156	4.4400	0.6547	-6.1653	1.4372	-0.4851	-1.5458	4.8811	0.2716
6	-3.2864	5.6593	-0.2053	-6.4110	2.4220	-1.6255	-1.0198	5.8612	-0.7779
8	-4.3041	5.7947	-1.1800	-6.9003	1.6994	-2.7377	-1.9985	6.0142	-1.7877
6	-1.9390	5.4634	-0.8795	-5.1078	3.1198	-1.9626	0.2825	5.3553	-1.3720
8	-1.6385	6.6693	-1.5535	-5.3744	4.0623	-2.9729	0.7330	6.3418	-2.2702
6	-0.8688	5.0728	0.1327	-4.5118	3.7637	-0.7182	1.2827	5.0627	-0.2628
8	0.3040	4.7022	-0.5865	-3.2085	4.1900	-1.0916	2.4245	4.4532	-0.8490

6	-1.3328	3.8828	0.9737	-4.3999	2.7505	0.4244	0.6562	4.0874	0.7361
8	-2.5897	4.2032	1.5779	-5.6666	2.1157	0.6463	-0.5664	4.6314	1.2351
6	-0.3721	3.5456	2.0971	-3.9883	3.3811	1.7394	1.5375	3.8442	1.9453
8	-0.2624	4.6448	2.9845	-4.9787	4.2983	2.1704	1.7557	5.0644	2.6278
6	1.0612	5.0242	3.2977	-4.4959	5.6025	2.4237	3.1068	5.3029	2.9860
6	1.6409	4.2897	4.5142	-3.8271	5.7949	3.8068	3.5241	4.6952	4.3375
6	1.3162	2.8018	4.5458	-3.5402	4.4982	4.5531	2.9547	3.2998	4.5881
8	3.0534	4.5117	4.4118	-2.6164	6.5184	3.5411	4.9416	4.7117	4.4067
6	1.2664	5.7151	-0.7376	-2.8650	5.5377	-0.9701	3.6003	5.2031	-0.9853
6	1.7524	5.6798	-2.1980	-2.1877	5.9737	-2.2708	4.1327	5.0054	-2.4077
8	0.6350	5.7255	-3.0725	-3.0667	5.7326	-3.3507	3.1905	5.4921	-3.3425
6	2.6063	4.4446	-2.4379	-0.8840	5.2113	-2.4487	4.3673	3.5222	-2.6239
8	3.1936	4.4961	-3.7125	-0.2678	5.7054	-3.6121	4.8787	3.3411	-3.9222
6	3.6729	4.3018	-1.3544	-0.0107	5.3955	-1.2145	5.2905	2.9520	-1.5557
8	4.2653	3.0457	-1.6362	1.1566	4.6109	-1.4127	5.1542	1.5382	-1.6686
6	3.0145	4.3059	0.0240	-0.7870	4.9599	0.0292	4.8351	3.3680	-0.1515
8	2.3184	5.5475	0.1737	-1.9820	5.7418	0.1089	4.5930	4.7725	-0.0794
6	3.9719	4.1505	1.2076	-0.0386	5.1800	1.3321	5.8441	2.9773	0.9160
8	3.5307	3.1017	2.0577	-0.7876	4.7137	2.4353	5.2627	2.9259	2.2045
6	5.6534	2.8877	-1.6348	2.3960	5.2696	-1.3682	6.2721	0.7071	-1.8581
6	5.9510	1.8638	-2.7294	3.2443	4.7798	-2.5466	5.9464	-0.2219	-3.0271
8	5.4610	2.3874	-3.9472	2.5153	4.9949	-3.7383	5.7055	0.5682	-4.1770
6	5.2697	0.5452	-2.3763	3.5975	3.3134	-2.3637	4.7279	-1.0649	-2.6809
8	5.6789	-0.4333	-3.3060	4.4528	2.9162	-3.4101	4.5319	-1.9869	-3.7284
6	5.5981	0.1346	-0.9460	4.2450	3.1262	-1.0049	4.9240	-1.7591	-1.3424
8	4.7283	-0.9488	-0.6446	4.4894	1.7384	-0.8858	3.6595	-2.3149	-1.0050
6	5.3668	1.2794	0.0415	3.3077	3.6448	0.0889	5.3753	-0.7694	-0.2636
8	6.1248	2.4066	-0.3937	3.0559	5.0318	-0.1502	6.5366	-0.0590	-0.7098
6	5.7223	0.9151	1.4676	3.8971	3.4848	1.4747	5.6592	-1.4453	1.0594
8	6.9755	0.2605	1.4903	5.2133	3.9894	1.4707	6.5067	-2.5551	0.8613
6	5.2642	-2.0280	0.0882	5.6632	1.3397	-0.2131	3.6770	-3.5732	-0.3732
6	5.2642	-3.2588	-0.8108	6.4705	0.4632	-1.1637	3.0938	-4.6131	-1.3275
8	6.0478	-2.9717	-1.9551	6.7133	1.2024	-2.3477	3.8036	-4.5397	-2.5508
6	3.8399	-3.5831	-1.2215	5.7048	-0.8076	-1.4976	1.6109	-4.3746	-1.5595
8	3.9031	-4.7791	-1.9725	6.5799	-1.6289	-2.2473	1.1588	-5.4262	-2.3759
6	2.9232	-3.6791	-0.0078	5.1699	-1.4988	-0.2437	0.8837	-4.3130	-0.2214
8	1.5729	-3.6533	-0.4719	4.1951	-2.4730	-0.6229	-0.4854	-4.0298	-0.5036
6	3.0885	-2.4773	0.9195	4.4531	-0.4879	0.6586	1.5423	-3.2049	0.6224
8	4.4770	-2.2769	1.2252	5.3360	0.6014	0.9358	2.9220	-3.5280	0.8114
6	2.3270	-2.6606	2.2167	4.0280	-1.0619	1.9990	0.9530	-2.8995	1.9995
8	2.7759	-3.8377	2.8510	5.1073	-1.7035	2.6473	1.2994	-3.7900	3.0381
6	1.7562	-4.6916	3.3365	4.9612	-3.1087	2.7245	0.6145	-5.0264	3.0290
6	2.2449	-6.1265	3.2586	6.3147	-3.7913	2.7781	1.5245	-6.1604	2.5415
6	1.2228	-7.0779	3.8694	6.1250	-5.2899	2.9876	2.3131	-6.7903	3.6804
8	2.4483	-6.4133	1.8787	6.9482	-3.5358	1.5298	0.6664	-7.1003	1.9033
1	1.6294	-5.7046	-0.2766	5.7317	-3.8300	-0.8661	-0.9553	-5.7293	0.5703

1	0.1498	-6.1436	-2.0944	4.5463	-5.1401	-2.5830	-3.0192	-6.1868	-0.5794
1	1.3681	-3.6647	-2.6094	4.1298	-3.3900	-4.1117	-2.1814	-6.1499	-2.8107
1	-0.8613	-3.2713	-2.0854	2.1822	-3.2500	-2.1768	-2.6465	-3.5536	-2.0790
1	-2.5870	-4.5437	-3.2107	1.2954	-5.0314	-3.5568	-4.6403	-4.2489	-2.9881
1	-2.1529	-5.6555	-0.6672	2.3573	-6.1807	-1.3527	-4.5487	-4.4772	0.1501
1	3.0561	-3.1805	-4.3569	2.4114	-3.5571	0.2510	-2.2793	-2.4146	-0.0005
1	-1.8344	-4.8966	2.2079	3.0281	-5.1810	2.1577	-2.9603	-2.4640	2.5893
1	-2.9098	-3.6639	1.5120	2.2871	-6.4689	1.1884	-4.5886	-2.7678	1.9339
1	-1.4621	-2.0972	2.2109	0.3369	-5.4493	1.3834	-4.1561	-0.7760	0.6075
1	-4.2871	-5.5098	-0.7037	0.4161	-6.9862	-0.9337	-6.2775	-4.2279	-1.1060
1	-6.2322	-4.4932	-1.9330	-1.7085	-7.0599	-2.1612	-7.8441	-2.6683	-2.3590
1	-5.0200	-4.2463	-3.9991	-0.8747	-6.1732	-4.1854	-6.2781	-2.5121	-4.1904
1	-4.2416	-2.2341	-2.4116	-1.4100	-4.0390	-2.5012	-5.4275	-0.8561	-2.4779
1	-6.1112	-1.2539	-3.3480	-3.6947	-4.5515	-3.2284	-6.9916	0.5569	-3.2397
1	-6.7895	-2.1062	-0.7255	-3.3718	-5.6490	-0.7889	-7.5288	0.2784	-0.8524
1	-3.8518	-2.1504	0.1623	-0.9932	-3.8468	-0.0726	-5.9586	-1.2920	1.0103
1	-4.8334	-0.9244	1.7795	-2.5319	-3.3694	1.5906	-3.4285	-1.1037	-1.8200
1	-4.8814	-2.5861	2.4134	-1.5580	-4.6954	2.2859	-8.9803	-1.0544	0.6183
1	-7.4735	-0.1666	-0.9132	-5.0474	-4.6254	-0.1789	-6.7840	1.9087	-0.0525
1	-7.2912	2.1111	-1.8020	-6.7790	-3.2249	-1.2115	-5.8252	3.6032	-1.3786
1	-6.2986	1.4829	-3.8633	-6.0754	-3.5178	-3.4619	-5.5197	2.5383	-3.4189
1	-4.2799	1.6125	-1.9360	-4.4913	-1.5606	-2.3602	-3.3153	1.9415	-1.8214
1	-4.6795	4.0796	-2.2461	-6.4369	-0.2522	-2.8685	-2.9080	4.4071	-2.4128
1	-5.8339	3.4797	-0.0781	-6.4953	-0.9680	-0.1180	-3.8964	4.2852	0.0436
1	-4.3255	0.8686	0.5140	-3.4630	-1.4346	-0.1050	-3.1764	1.3308	0.3977
1	-4.2541	2.4973	2.3842	-3.7784	0.2416	1.4964	-1.9965	2.7284	2.0886
1	-5.2350	1.0633	2.7645	-3.8319	-1.2765	2.4084	-3.3004	1.7275	2.8014
1	-7.0454	2.2626	2.5908	-5.8215	0.5865	1.9598	-4.5474	3.5317	2.9596
1	-4.5371	4.5990	1.2393	-7.1073	0.9629	-0.1673	-2.3971	5.3108	0.8214
1	-3.2393	6.5507	0.4450	-7.1486	3.1714	-1.2862	-0.8248	6.8266	-0.2765
1	-4.0019	6.4778	-1.7942	-6.7958	2.2736	-3.5082	-1.5627	6.4826	-2.5135
1	-2.0410	4.6238	-1.5949	-4.3912	2.3515	-2.3125	0.0764	4.4000	-1.8970
1	-0.9356	6.4960	-2.2005	-4.5385	4.5050	-3.2012	1.4936	5.9868	-2.7617
1	-0.6537	5.9165	0.8131	-5.1321	4.6206	-0.3976	1.5615	5.9911	0.2668
1	-1.4357	2.9921	0.3271	-3.6409	1.9978	0.1421	0.4617	3.1235	0.2246
1	0.6089	3.2883	1.6593	-3.0206	3.8911	1.5927	2.4949	3.4070	1.6109
1	-0.7412	2.6520	2.6238	-3.8421	2.5887	2.4953	1.0466	3.1076	2.6032
1	0.8235	6.6988	-0.5183	-3.7547	6.1544	-0.7626	3.4171	6.2676	-0.7711
1	2.3516	6.5802	-2.3957	-1.9555	7.0511	-2.1913	5.0882	5.5522	-2.4959
1	0.2443	4.8408	-3.0733	-2.5402	5.7929	-4.1591	3.3916	5.0725	-4.1899
1	1.9484	3.5527	-2.3368	-1.1181	4.1314	-2.5429	3.3874	3.0173	-2.5096
1	3.7938	3.7336	-3.7801	0.6012	5.2782	-3.7068	5.0093	2.3867	-4.0620
1	4.4175	5.1144	-1.4357	0.2577	6.4635	-1.1146	6.3330	3.2614	-1.7508
1	2.2961	3.4633	0.0583	-1.0566	3.8884	-0.0605	3.8929	2.8385	0.0571
1	3.9989	5.1084	1.7517	0.2029	6.2516	1.4371	6.6570	3.7166	0.9410
1	4.9910	3.9334	0.8503	0.9114	4.6264	1.2944	6.2758	1.9969	0.6443

1	6.1663	3.8442	-1.8202	2.2540	6.3593	-1.4319	7.1717	1.3084	-2.0596
1	7.0419	1.7002	-2.7724	4.1814	5.3650	-2.5520	6.8096	-0.8917	-3.1868
1	5.5364	1.6953	-4.6159	2.9909	4.5528	-4.4529	5.3374	-0.0168	-4.8518
1	4.1736	0.7075	-2.4519	2.6557	2.7267	-2.3780	3.8549	-0.3883	-2.5847
1	5.6782	-1.3021	-2.8650	5.0330	2.2083	-3.0775	4.0558	-2.7547	-3.3674
1	6.6528	-0.1862	-0.8942	5.1928	3.6907	-0.9621	5.6795	-2.5565	-1.4546
1	4.2945	1.5492	0.0442	2.3570	3.0805	0.0491	4.5687	-0.0520	-0.0659
1	4.9201	0.2690	1.8623	3.9003	2.4091	1.7274	4.6885	-1.7713	1.4785
1	5.7376	1.8335	2.0794	3.2668	4.0132	2.2138	6.1022	-0.7147	1.7605
1	6.2733	-1.7780	0.4485	6.2421	2.2134	0.1242	4.7026	-3.8506	-0.0837
1	5.6882	-4.1082	-0.2475	7.4188	0.1953	-0.6643	3.2173	-5.6107	-0.8660
1	5.8905	-3.6943	-2.5791	7.0695	0.5709	-2.9877	3.3422	-5.1217	-3.1698
1	3.4770	-2.7370	-1.8418	4.8389	-0.5119	-2.1149	1.4876	-3.3924	-2.0607
1	3.0463	-4.9197	-2.4070	6.0308	-2.1917	-2.8155	0.1863	-5.4161	-2.3890
1	3.1162	-4.6037	0.5632	5.9897	-1.9753	0.3200	0.9623	-5.2974	0.2701
1	2.6987	-1.5884	0.4083	3.5506	-0.1127	0.1422	1.4547	-2.2622	0.0437
1	1.2489	-2.7140	1.9762	3.1801	-1.7520	1.8410	-0.1467	-2.8122	1.8938
1	2.4889	-1.7795	2.8639	3.6699	-0.2331	2.6301	1.3449	-1.9230	2.3134
1	1.7227	4.8462	2.4340	-3.7527	5.8938	1.6605	3.7798	4.9116	2.2036
1	1.0574	6.1060	3.4926	-5.3607	6.2721	2.3288	3.2403	6.3940	3.0243
1	1.2667	4.7590	5.4396	-4.4759	6.4285	4.4340	3.1762	5.3528	5.1508
1	1.8377	2.3182	5.3822	-3.1590	4.7208	5.5584	3.3804	2.8977	5.5161
1	0.2390	2.6485	4.6854	-4.4568	3.9039	4.6562	1.8631	3.3392	4.6991
1	1.6229	2.3082	3.6113	-2.7910	3.8824	4.0347	3.1799	2.5977	3.7710
1	3.4705	4.2488	5.2401	-2.2248	6.7798	4.3831	5.2471	4.1243	3.6956
1	-7.1916	-2.4866	3.7045	-3.5224	-5.3366	3.7257	-7.1324	-0.0544	3.4876
1	-6.2503	-0.9679	3.6483	-4.1558	-3.8221	3.0209	-5.9555	0.4455	2.2247
1	-9.1161	-1.2368	2.6380	-5.4593	-6.5646	2.6537	-7.1053	2.6821	2.1153
1	-9.6520	0.2347	4.6031	-7.2089	-5.6491	4.2070	-8.4660	3.4097	4.0671
1	-9.0216	-1.3431	5.1316	-5.6386	-5.7965	5.0329	-9.2393	2.0126	3.2703
1	-7.9686	0.0970	5.1604	-6.2114	-4.2030	4.4801	-8.3390	1.7820	4.7850
1	-7.6047	0.3634	1.7129	-6.0561	-3.9713	1.7739	-5.9292	2.1017	4.6164
1	1.5007	-4.4431	4.3825	4.3687	-3.3888	3.6157	0.2738	-5.2350	4.0566
1	0.8460	-4.5947	2.7205	4.4470	-3.4856	1.8264	-0.2862	-4.9659	2.3972
1	3.2054	-6.2007	3.8015	6.9099	-3.3561	3.6018	2.2343	-5.7204	1.8160
1	1.5589	-8.1193	3.7826	7.0918	-5.8100	2.9881	3.0041	-7.5602	3.3121
1	1.0625	-6.8618	4.9334	5.6257	-5.5029	3.9417	2.9038	-6.0219	4.1969
1	0.2635	-6.9816	3.3420	5.5153	-5.6941	2.1661	1.6286	-7.2511	4.4058
1	2.8607	-7.2811	1.8101	7.8261	-3.9319	1.5487	1.1982	-7.8462	1.6040
1	3.5219	3.4439	2.9672	-1.4358	5.3945	2.6946	4.6053	2.2094	2.1799
6	7.4908	0.0241	2.7905	5.9570	3.5681	2.5952	6.4819	-3.4580	1.9457
6	6.9997	-1.2852	3.4061	7.3996	3.9984	2.4093	7.1768	-4.7398	1.5255
6	7.7010	-1.5405	4.7334	8.2239	3.7090	3.6583	7.3202	-5.6987	2.7015
8	5.5994	-1.2424	3.6478	7.8893	3.2719	1.2893	6.3740	-5.3037	0.4958
1	8.5864	-0.0047	2.6932	5.5459	4.0041	3.5240	6.9756	-3.0246	2.8343
1	7.2268	0.8607	3.4637	5.9182	2.4641	2.6810	5.4326	-3.6957	2.2169

1	7.2356	-2.1038	2.6999	7.4086	5.0823	2.1921	8.1736	-4.4749	1.1281
1	7.3503	-2.4833	5.1687	9.2755	3.9786	3.4968	7.7854	-6.6387	2.3781
1	8.7899	-1.5940	4.6096	7.8563	4.2820	4.5190	7.9457	-5.2669	3.4931
1	7.4708	-0.7308	5.4400	8.1784	2.6389	3.9020	6.3323	-5.9322	3.1212
1	5.1459	-1.6369	2.8897	8.7734	3.5934	1.0825	6.8370	-6.0659	0.1323
6	1.5866	0.7216	0.7814	-0.2928	-2.4359	3.1262	-0.3830	0.0771	3.0403
7	0.3510	0.4729	1.1486	-0.9927	-1.4330	3.5956	0.8697	0.4343	2.8848
6	-0.2321	-0.1658	0.0792	-0.9237	-0.4560	2.6306	1.0339	0.5906	1.5292
6	0.6918	-0.3203	-0.9433	-0.1610	-0.9030	1.5569	-0.1642	0.3309	0.8747
7	1.8345	0.2710	-0.4841	0.2253	-2.1716	1.8927	-1.0516	-0.0053	1.8539
6	-1.6761	-0.4997	0.0828	-1.4919	0.8988	2.8624	2.3469	0.8813	0.9213
8	-2.2985	-0.6807	1.1387	-2.1513	1.1589	3.8676	3.3747	0.9696	1.6111
7	-2.2665	-0.5558	-1.1247	-1.2280	1.8223	1.9037	2.3540	1.0252	-0.4180
7	0.5361	-0.9449	-2.1728	0.1240	-0.1888	0.4087	-0.4279	0.4834	-0.4751
7	1.6588	-1.1625	-2.7284	1.0084	-0.6861	-0.3556	-1.5001	-0.0807	-0.8597
7	1.6071	-1.7052	-3.9100	1.2160	0.0288	-1.4260	-1.8022	0.1423	-2.1010
6	2.8774	-2.1010	-4.4935	2.2060	-0.4270	-2.3786	-2.9658	-0.5322	-2.6334
6	0.3479	-1.9681	-4.5860	0.4129	1.2011	-1.7133	-1.0320	1.0679	-2.9070
1	2.3360	1.2566	1.3669	-0.1079	-3.3858	3.6179	-0.8685	-0.1419	3.9856
1	2.7366	0.2087	-0.9460	0.7534	-2.8488	1.3507	-2.0091	-0.3493	1.7036
1	-1.7325	-0.4071	-1.9707	-0.5918	1.5711	1.1553	1.4924	0.9328	-0.9455
1	-3.2742	-0.6476	-1.1839	-1.2940	2.8025	2.1702	3.2309	1.1726	-0.9056
1	-0.7272	-3.0478	0.1082	1.7269	-0.7703	-3.3070	-3.6913	0.2041	-3.0128
1	2.8722	-1.8781	-5.5661	2.8927	0.3999	-2.6164	-2.6815	-1.2118	-3.4487
1	3.6790	-1.5301	-4.0099	2.7754	-1.2472	-1.9271	-8.1564	-1.6454	2.0898
1	-0.1739	-2.8407	-4.1630	0.6379	1.5264	-2.7337	-1.5630	1.2212	-3.8506
1	-0.3005	-1.0885	-4.4919	-0.6540	0.9548	-1.6223	-0.9371	2.0208	-2.3603
1	0.5680	-2.1615	-5.6392	0.6325	2.0263	-1.0148	-0.0240	0.6770	-3.1049

HE-β-CD:DTIC

Atomic Number	**K04_01**			**K03_02**			**K03_03**		
	x	**y**	**z**	**x**	**y**	**z**	**x**	**y**	**z**
6	-1.0737	-5.7276	-0.3264	1.2772	5.2684	-0.3508	-0.4645	5.7005	-0.7967
6	-1.7139	-5.8597	-1.7055	0.8487	5.6550	1.0762	0.1130	5.4220	-2.1895
8	-0.7148	-6.0231	-2.6895	1.9532	5.5692	1.9622	-0.9088	4.8700	-3.0103
6	-2.4982	-4.5924	-1.9881	-0.3031	4.7766	1.5376	1.2720	4.4439	-2.0637
8	-3.0771	-4.7488	-3.2683	-0.7700	5.2409	2.7767	1.8969	4.2964	-3.3107
6	-3.5111	-4.3020	-0.8892	-1.4034	4.8147	0.4863	2.2545	4.8727	-0.9819
8	-3.9837	-2.9610	-1.0522	-2.4296	3.9518	0.9416	3.1276	3.7562	-0.8392
6	-2.8581	-4.3969	0.4992	-0.8832	4.3903	-0.8869	1.5412	5.1650	0.3412
8	-2.1095	-5.6042	0.6207	0.1895	5.2692	-1.2400	0.5176	6.1406	0.1102
6	-3.8812	-4.3942	1.6374	-1.9649	4.5013	-1.9764	2.4705	5.6921	1.4418
8	-4.3211	-3.0902	1.9459	-2.5350	3.2561	-2.3076	2.9840	4.6500	2.2445
6	-5.1148	-2.7579	-1.8782	-3.7256	4.4619	1.0919	4.4963	3.9653	-0.6246
6	-4.7545	-1.6744	-2.9015	-4.2777	3.9100	2.4090	5.2719	3.4428	-1.8344
8	-3.5476	-2.0184	-3.5717	-3.4189	4.3071	3.4577	4.7687	4.0982	-2.9813
6	-4.5839	-0.3167	-2.2304	-4.3755	2.3968	2.3139	5.1031	1.9371	-1.9572

8	-4.5322	0.6991	-3.2053	-4.9796	1.9231	3.4950	5.9369	1.5092	-3.0047
6	-5.6189	-0.0163	-1.1423	-5.1756	2.0197	1.0769	5.4526	1.2732	-0.6341
8	-4.9828	0.9699	-0.3380	-5.1107	0.5980	1.0053	5.2025	-0.1196	-0.7761
6	-5.9737	-1.2445	-0.2883	-4.5684	2.6627	-0.1678	4.5950	1.8679	0.4829
8	-6.2269	-2.3730	-1.1250	-4.5595	4.0804	0.0232	4.8931	3.2764	0.5426
6	-7.2445	-1.0378	0.5327	-5.2828	2.3333	-1.4642	4.8694	1.2533	1.8406
8	-7.0209	-0.1249	1.5881	-6.6888	2.3275	-1.3248	6.2574	1.0984	2.0165
6	-6.7652	-0.7642	2.8318	-7.3124	2.2784	-2.6030	6.6166	0.8826	3.3723
6	-6.3129	0.3024	3.8089	-8.6606	1.5999	-2.4717	8.0026	0.2706	3.3687
8	-5.0678	0.8575	3.4410	-8.5119	0.2345	-2.1247	7.9884	-1.0120	2.7813
6	-5.6694	2.1267	0.0631	-6.3202	-0.0980	0.8702	6.3042	-0.9892	-0.7129
6	-5.6874	3.1996	-1.0323	-6.2790	-1.3065	1.7948	6.1789	-2.0184	-1.8297
8	-6.3336	2.6859	-2.1875	-6.0816	-0.8314	3.1136	6.1597	-1.3436	-3.0718
6	-4.2750	3.6425	-1.3724	-5.1482	-2.2254	1.3704	4.9053	-2.8222	-1.6386
8	-4.3753	4.7118	-2.2838	-5.2149	-3.3834	2.1657	4.8884	-3.8131	-2.6370
6	-3.5553	4.0524	-0.1014	-5.1913	-2.5475	-0.1248	4.7905	-3.4118	-0.2318
8	-2.2311	4.3926	-0.4835	-3.8880	-3.0297	-0.4070	3.4222	-3.8001	-0.1352
6	-3.5808	2.9107	0.9094	-5.4305	-1.2969	-0.9764	5.1285	-2.3519	0.8321
8	-4.9733	2.6257	1.1816	-6.5085	-0.5298	-0.4499	6.3439	-1.6690	0.5148
6	-2.8715	3.2532	2.2174	-5.7746	-1.5833	-2.4323	5.3068	-2.8686	2.2528
8	-3.0421	4.6068	2.5980	-7.0089	-2.2466	-2.5607	4.1753	-3.5710	2.6965
6	-1.7119	5.6038	-0.0223	-3.6928	-4.1317	-1.2533	3.1029	-5.0275	0.4745
6	-1.0480	6.3172	-1.2008	-3.2737	-5.3229	-0.3945	2.6233	-6.0234	-0.5872
8	-2.0055	6.4453	-2.2329	-4.2984	-5.5908	0.5436	3.6219	-6.1392	-1.5847
6	0.1690	5.5367	-1.6673	-1.9898	-4.9685	0.3404	1.3090	-5.5726	-1.2057
8	0.7973	6.2953	-2.6719	-1.6343	-6.0966	1.1168	0.8837	-6.6051	-2.0699
6	1.0865	5.2897	-0.4793	-0.9116	-4.5244	-0.6477	0.2910	-5.2663	-0.1189
8	2.1842	4.5278	-0.9499	0.2135	-4.0132	0.0651	-0.8505	-4.6735	-0.7268
6	0.3187	4.5496	0.6159	-1.4644	-3.3904	-1.5211	0.8923	-4.2802	0.8750
8	-0.7772	5.3877	1.0155	-2.6698	-3.8267	-2.1605	2.0886	-4.8319	1.4187
6	1.1572	4.2479	1.8352	-0.5017	-2.9474	-2.6051	-0.0332	-3.9927	2.0321
8	1.7719	5.4283	2.2917	-0.1565	-4.0351	-3.4429	-0.2953	-5.1915	2.7289
6	2.7990	5.1780	3.2348	1.2329	-4.3076	-3.4690	-1.4934	-5.1354	3.4750
6	2.3896	4.2997	4.4167	2.0128	-3.2454	-4.2435	-1.5517	-4.0014	4.4960
8	2.5091	2.9071	4.1542	3.3671	-3.6234	-4.3817	-1.9362	-2.7515	3.9336
6	3.4695	5.0476	-0.7499	1.1042	-4.9879	0.5710	-1.9838	-5.4878	-0.8525
6	4.2559	4.8593	-2.0538	1.3491	-4.6386	2.0521	-2.5602	-5.2433	-2.2564
8	3.5505	5.4951	-3.1013	0.0977	-4.4577	2.6993	-1.5563	-5.4782	-3.2325
6	4.4116	3.3743	-2.3188	2.2077	-3.3844	2.1798	-3.1142	-3.8309	-2.3373
8	5.1674	3.1930	-3.4939	2.5952	-3.2112	3.5181	-3.7451	-3.6367	-3.5766
6	5.0677	2.7034	-1.1228	3.4166	-3.4735	1.2522	-4.0810	-3.5957	-1.1832
8	5.0223	1.3173	-1.4086	4.0908	-2.2218	1.3435	-4.4303	-2.2243	-1.2587
6	4.2645	2.9923	0.1472	2.9560	-3.7517	-0.1746	-3.4255	-3.8869	0.1655
8	4.1244	4.4056	0.3152	2.2964	-5.0151	-0.1683	-2.9243	-5.2259	0.1604
6	4.9102	2.4171	1.4118	4.0808	-3.7879	-1.2092	-4.4058	-3.7383	1.3441
8	3.9968	1.6852	2.2102	4.1723	-2.5749	-1.9429	-4.1246	-2.6296	2.1663

6	6.1895	0.5524	-1.3714	5.4862	-2.2009	1.4963	-5.7683	-1.8329	-1.3001
6	6.0385	-0.4986	-2.4718	5.8233	-1.2100	2.6077	-5.8559	-0.7033	-2.3230
8	5.8695	0.1888	-3.6961	5.1038	-1.5894	3.7624	-5.4462	-1.2124	-3.5755
6	4.8292	-1.3676	-2.1467	5.4448	0.1905	2.1655	-4.9471	0.4409	-1.8819
8	4.7145	-2.3911	-3.1101	5.8878	1.0780	3.1675	-5.0541	1.4954	-2.8141
6	4.9497	-1.9302	-0.7372	6.0236	0.5522	0.8001	-5.2951	0.8632	-0.4622
8	3.7192	-2.5882	-0.4785	5.4015	1.8052	0.5425	-4.2623	1.7489	-0.0310
6	5.1860	-0.8021	0.2705	5.6984	-0.5439	-0.2284	-5.3286	-0.3451	0.4830
8	6.3542	-0.0788	-0.1207	6.1238	-1.8159	0.3047	-6.2008	-1.3489	-0.0436
6	5.3723	-1.2885	1.6901	6.4125	-0.3995	-1.5711	-5.8170	0.0226	1.8691
8	6.4055	-2.2504	1.7159	7.7693	-0.0284	-1.4267	-7.0512	0.7078	1.7522
6	3.7645	-3.7244	0.3544	5.7048	2.5007	-0.6321	-4.6527	2.9180	0.6769
6	3.4756	-4.9635	-0.4930	5.6492	3.9912	-0.3175	-4.7289	4.0949	-0.2983
8	4.3508	-4.9449	-1.6058	6.6016	4.3047	0.6676	-5.6881	3.8095	-1.3000
6	2.0293	-4.9829	-0.9642	4.2493	4.3487	0.1668	-3.3612	4.3202	-0.9247
8	1.8354	-6.2190	-1.6108	4.2507	5.7474	0.3855	-3.4722	5.4244	-1.7966
6	1.0702	-4.7497	0.1996	3.1957	3.9034	-0.8448	-2.3291	4.5286	0.1746
8	-0.2422	-4.5975	-0.3230	1.8884	4.0005	-0.2802	-1.0251	4.4834	-0.3785
6	1.4821	-3.4466	0.8860	3.4079	2.4342	-1.2369	-2.3822	3.3682	1.1616
8	2.8167	-3.5949	1.3762	4.7596	2.2237	-1.6454	-3.7059	3.1815	1.6692
6	0.5894	-3.0171	2.0227	2.5057	2.0333	-2.3857	-1.4153	3.5539	2.3186
8	0.5934	-3.9957	3.0392	2.7198	2.9089	-3.4679	-1.4024	4.9060	2.7091
6	0.0834	-3.5267	4.2714	1.7740	2.7252	-4.5043	-0.4631	5.1727	3.7347
6	-1.4362	-3.4863	4.3138	0.3576	3.1287	-4.0762	-0.4755	6.6746	3.9369
8	-1.9911	-2.5815	3.3658	-0.5231	2.0390	-3.8284	-0.0418	7.3558	2.7761
1	-0.5068	-6.6327	-0.0588	1.9878	6.0099	-0.7457	-1.2285	6.4916	-0.8369
1	-2.3948	-6.7290	-1.6869	0.5207	6.7048	1.0796	0.4513	6.3560	-2.6582
1	-1.1305	-5.8480	-3.5449	2.1016	4.6295	2.1361	-1.0243	3.9590	-2.6931
1	-1.7726	-3.7593	-1.9708	0.0597	3.7279	1.6050	0.8426	3.4786	-1.7091
1	-3.3038	-3.8691	-3.6143	-1.5804	4.7494	2.9957	2.8112	4.0005	-3.1598
1	-4.3579	-5.0080	-0.9553	-1.7828	5.8512	0.4087	2.8165	5.7628	-1.3208
1	-2.1816	-3.5318	0.6338	-0.5225	3.3410	-0.8512	1.0852	4.2293	0.7102
1	-3.4093	-4.8783	2.5084	-1.5124	4.9939	-2.8544	1.8737	6.3470	2.0907
1	-4.7575	-4.9992	1.3596	-2.7859	5.1437	-1.6233	3.2761	6.3102	1.0046
1	-3.6435	-2.7256	2.5389	-1.9046	2.7803	-2.8778	3.6643	4.1707	1.7500
1	-5.3813	-3.6983	-2.3837	-3.7152	5.5631	1.1021	4.7150	5.0309	-0.4522
1	-5.5494	-1.6187	-3.6574	-5.2929	4.3201	2.5561	6.3429	3.6686	-1.6883
1	-2.8266	-1.8231	-2.9505	-3.6568	3.7884	4.2371	5.1820	3.6762	-3.7469
1	-3.6074	-0.3430	-1.7026	-3.3513	1.9831	2.1978	4.0362	1.7255	-2.1773
1	-5.1739	1.3874	-2.9662	-5.2119	0.9876	3.3702	5.8329	0.5484	-3.1156
1	-6.5384	0.3778	-1.6098	-6.2227	2.3476	1.1891	6.5131	1.4479	-0.3890
1	-5.1486	-1.4803	0.4044	-3.5245	2.3288	-0.2871	3.5244	1.7393	0.2529
1	-7.5783	-2.0161	0.9161	-4.9481	1.3342	-1.8090	4.3506	0.2759	1.9139
1	-8.0457	-0.6366	-0.1079	-4.9519	3.0642	-2.2192	4.4393	1.9121	2.6172
1	-6.6880	1.8842	0.4022	-7.1689	0.5596	1.1091	7.2447	-0.4243	-0.7949
1	-6.2453	4.0671	-0.6374	-7.2403	-1.8405	1.7067	7.0480	-2.6962	-1.7634

1	-6.3254	3.3951	-2.8451	-6.0195	-1.5997	3.6956	5.8639	-1.9776	-3.7381
1	-3.7380	2.7813	-1.8189	-4.1950	-1.6811	1.5479	4.0485	-2.1284	-1.7608
1	-3.4962	5.1201	-2.3689	-4.7419	-4.0978	1.7055	4.2597	-4.5061	-2.3700
1	-4.0604	4.9264	0.3447	-5.9640	-3.3098	-0.3298	5.4559	-4.2901	-0.1440
1	-3.1096	2.0125	0.4757	-4.4986	-0.7063	-0.9493	4.2905	-1.6406	0.8537
1	-1.8029	3.0001	2.1037	-4.9795	-2.2110	-2.8652	5.5481	-1.9996	2.8941
1	-3.2662	2.5922	3.0039	-5.7735	-0.6263	-2.9838	6.1716	-3.5494	2.2956
1	-2.2055	5.0510	2.4088	-7.6960	-1.5630	-2.5490	3.3828	-3.0796	2.4247
1	-2.5075	6.2300	0.4107	-4.6003	-4.3527	-1.8384	3.9697	-5.4201	1.0247
1	-0.7107	7.3110	-0.8546	-3.1008	-6.1949	-1.0490	2.4603	-6.9962	-0.0890
1	-1.5262	6.7176	-3.0265	-3.9316	-6.2443	1.1567	3.2431	-6.6857	-2.2871
1	-0.1697	4.5552	-2.0552	-2.2178	-4.1052	0.9955	1.4965	-4.6343	-1.7652
1	1.6383	5.8628	-2.9015	-1.1516	-5.7776	1.8953	0.1053	-6.2936	-2.5611
1	1.4338	6.2527	-0.0669	-0.6029	-5.3644	-1.2965	0.0085	-6.1872	0.4200
1	-0.0745	3.5926	0.2242	-1.6785	-2.5191	-0.8745	1.1134	-3.3332	0.3517
1	1.9140	3.4824	1.5710	0.3864	-2.5047	-2.1216	-0.9685	-3.5555	1.6356
1	0.4948	3.8130	2.6043	-0.9822	-2.1543	-3.1997	0.4514	-3.2415	2.6809
1	3.4191	6.1131	-0.4779	0.6662	-5.9909	0.4800	-1.7095	-6.5491	-0.7425
1	5.2546	5.3134	-1.9226	1.8522	-5.4798	2.5488	-3.3729	-5.9633	-2.4375
1	3.9069	5.1495	-3.9303	-0.3088	-3.6909	2.2656	-1.1460	-4.6302	-3.4435
1	3.3988	2.9402	-2.4301	1.5819	-2.5350	1.8295	-2.2688	-3.1224	-2.1997
1	5.2493	2.2354	-3.6421	3.2815	-2.5222	3.5447	-4.1581	-2.7557	-3.5634
1	6.1119	3.0499	-1.0137	4.0842	-4.2869	1.5882	-4.9743	-4.2335	-1.3160
1	3.2664	2.5307	0.0168	2.2292	-2.9759	-0.4806	-2.5965	-3.1645	0.3052
1	5.3677	3.2456	1.9754	3.8755	-4.6206	-1.9028	-4.4017	-4.6868	1.9084
1	5.7173	1.7264	1.1268	5.0549	-3.9779	-0.7308	-5.4281	-3.5890	0.9649
1	7.0827	1.1771	-1.5281	5.8572	-3.2086	1.7377	-6.4290	-2.6748	-1.5578
1	6.9462	-1.1272	-2.4888	6.9136	-1.2428	2.7869	-6.8992	-0.3436	-2.3631
1	5.6151	-0.4612	-4.3629	5.1959	-0.8738	4.4049	-5.3352	-0.4570	-4.1677
1	3.9412	-0.7078	-2.1744	4.3411	0.2385	2.0745	-3.9030	0.0680	-1.8827
1	4.3728	-3.1863	-2.6659	5.6866	1.9718	2.8610	-5.3120	2.3084	-2.3461
1	5.7883	-2.6484	-0.6980	7.1192	0.6635	0.8680	-6.2738	1.3728	-0.4475
1	4.3061	-0.1321	0.2617	4.6085	-0.5662	-0.4159	-4.3193	-0.7785	0.5739
1	4.4203	-1.7302	2.0403	5.9108	0.3764	-2.1617	-5.0614	0.6699	2.3555
1	5.6078	-0.4300	2.3444	6.3036	-1.3558	-2.1052	-5.9105	-0.9013	2.4582
1	4.7509	-3.7986	0.8404	6.6905	2.2017	-1.0249	-5.6174	2.7440	1.1811
1	3.6508	-5.8591	0.1299	5.8451	4.5363	-1.2605	-5.0242	4.9933	0.2717
1	4.0604	-5.6605	-2.1881	6.3652	5.1877	0.9828	-5.6182	4.5259	-1.9478
1	1.8832	-4.1370	-1.6693	4.0718	3.8035	1.1132	-3.0848	3.3969	-1.4765
1	1.0305	-6.1592	-2.1516	3.5671	5.9413	1.0465	-2.7307	5.3893	-2.4223
1	1.1111	-5.5795	0.9267	3.2644	4.5277	-1.7525	-2.5040	5.4860	0.6924
1	1.4385	-2.6348	0.1371	3.1752	1.7924	-0.3666	-2.0651	2.4741	0.6045
1	-0.4229	-2.8461	1.6240	1.4626	2.0925	-2.0111	-0.4064	3.2403	1.9956
1	0.9628	-2.0507	2.4146	2.7011	0.9887	-2.6783	-1.7213	2.8983	3.1537
1	3.6615	4.7072	2.7264	1.6240	-4.4052	-2.4379	-2.3569	-5.0442	2.7861
1	3.1136	6.1644	3.6013	1.3605	-5.2797	-3.9660	-1.5734	-6.0995	3.9954

1	1.3681	4.5572	4.7407	1.9189	-2.2653	-3.7398	-0.5818	-3.9187	5.0127
1	1.6921	2.5276	3.7814	3.8464	-3.2020	-3.6510	-1.1792	-2.3043	3.5204
1	-7.6822	-1.2613	3.1961	-7.4130	3.2961	-3.0174	6.5890	1.8334	3.9326
1	-5.9790	-1.5330	2.7144	-6.6916	1.6869	-3.3010	5.9066	0.1809	3.8479
1	-6.1934	-0.1474	4.8041	-9.1907	1.6481	-3.4318	8.3649	0.1651	4.4005
1	-5.1798	1.3524	2.6130	-7.9027	0.1990	-1.3715	7.4708	-0.9583	1.9630
1	0.4393	-4.2170	5.0492	2.1170	3.3567	-5.3334	-0.7379	4.6451	4.6650
1	0.4963	-2.5245	4.4958	1.7673	1.6756	-4.8535	0.5436	4.8267	3.4244
1	-1.7712	-3.2469	5.3362	-0.1239	3.7143	-4.8706	0.1962	6.9478	4.7621
1	-1.7527	-1.6697	3.5844	-0.1825	1.4283	-3.1511	-0.3312	6.8483	2.0032
1	3.6276	2.2438	2.9207	3.4423	-1.9739	-1.7071	-3.3515	-2.8162	2.7287
6	6.5790	-2.8311	2.9974	8.7124	-1.0888	-1.3933	-8.0256	0.3702	2.7313
6	7.8334	-3.6783	2.9018	9.5803	-0.9793	-0.1524	-8.9136	-0.7556	2.2221
8	8.9319	-2.8780	2.5130	8.8152	-1.0731	1.0355	-8.1796	-1.9373	1.9690
1	6.7106	-2.0376	3.7546	8.1916	-2.0622	-1.3929	-7.5363	0.0777	3.6749
1	5.6962	-3.4359	3.2739	9.3458	-1.0492	-2.2947	-8.6268	1.2705	2.9229
1	7.6617	-4.5008	2.1842	10.0921	-0.0059	-0.1407	-9.4415	-0.4123	1.3151
1	8.6216	-2.3620	1.7577	8.0635	-1.6498	0.8445	-7.6338	-1.7840	1.1841
1	3.0648	4.5190	5.2558	1.5647	-3.1431	-5.2445	-2.3114	-4.2485	5.2501
1	8.0670	-4.1240	3.8775	10.3563	-1.7643	-0.1957	-9.6752	-0.9922	2.9792
1	-1.8269	-4.4791	4.0532	0.4607	3.7886	-3.1932	-1.4988	6.9820	4.2179
1	-7.0943	1.0791	3.8842	-9.2713	2.1305	-1.7208	8.6922	0.9539	2.8395
6	-2.9389	-0.4069	1.6226	-1.9563	0.3353	-1.3144	-1.8409	-0.4893	1.8416
7	-2.0102	0.2655	2.2600	-0.6885	0.2083	-1.6263	-0.6332	-0.9319	2.1078
6	-0.8827	0.1670	1.4827	-0.0593	-0.1757	-0.4658	0.1431	-0.5766	1.0308
6	-1.1570	-0.5929	0.3498	-0.9859	-0.2866	0.5602	-0.6388	0.1066	0.1073
7	-2.4719	-0.9523	0.4669	-2.1886	0.0388	-0.0038	-1.8951	0.1368	0.6396
6	0.3855	0.7967	1.9244	1.3822	-0.4734	-0.4027	1.5952	-0.8947	0.9629
8	0.4151	1.4603	2.9700	2.0243	-0.8164	-1.4086	2.1765	-1.4603	1.8936
7	1.4647	0.5927	1.1503	1.9469	-0.3495	0.8097	2.2009	-0.5184	-0.1812
7	-0.2751	-0.9109	-0.6685	-0.7702	-0.6472	1.8785	-0.2634	0.6458	-1.1160
7	-0.7618	-1.5496	-1.6510	-1.8512	-0.6084	2.5558	-1.2153	1.1974	-1.7357
7	0.1192	-1.8645	-2.5705	-1.7307	-0.9132	3.8031	-0.8819	1.7388	-2.8941
6	-0.3999	-2.3095	-3.8547	-2.9320	-0.8406	4.6122	-1.9905	1.9185	-3.8271
6	1.4679	-1.3319	-2.4994	-0.4415	-1.2287	4.3882	0.4269	1.4714	-3.4745
1	-3.9717	-0.4958	1.9476	-2.7445	0.6571	-1.9892	-2.7150	-0.6036	2.4765
1	-2.9818	-1.5974	-0.1395	-3.0808	0.0774	0.4896	-2.6999	0.6255	0.2437
1	1.3837	0.0422	0.3028	1.3593	-0.1814	1.6190	1.6741	-0.0395	-0.9033
1	2.3704	0.9466	1.4603	2.8592	-0.7681	0.9586	3.2007	-0.6234	-0.3034
1	-0.8097	-1.4719	-4.4384	-3.0814	-1.7862	5.1472	-1.8308	2.8330	-4.4121
1	0.4188	-2.7670	-4.4163	-2.8585	-0.0212	5.3394	-2.0492	1.0636	-4.5175
1	-1.1736	-3.0721	-3.7172	-3.7765	-0.6625	3.9382	-2.9328	1.9800	-3.2700
1	2.0511	-1.7387	-3.3317	-0.5879	-1.4080	5.4560	0.5365	2.1046	-4.3593
1	1.4508	-0.2307	-2.5499	-0.0010	-2.1219	3.9196	1.2225	1.7172	-2.7633
1	1.9485	-1.6261	-1.5585	0.2516	-0.3893	4.2386	0.5115	0.4076	-3.7473

Table S3. Densities, viscosities and relative permittivities of pure water at temperatures T = (288.15 to 318.15)K.

T/K	ρ_0 /kg·m^{-3} [a]	$10^3 \cdot \eta$ /Pa·s [a]	ε_r [b]
283.15	999.700	1.130	83.95
288.15	999.100	1.138	82.07
293.15	998.205	1.002	80.21
298.15	997.047	0.890	78.40
303.15	995.651	0.797	76.62
308.15	994.038	0.719	74.89
313.15	992.224	0.653	73.19
318.15	990.223	0.596	71.53

[a] values for water recommended by the International Association for the Properties of Water and Steam (IAPWS) calculated on the online property calculator (https://web1.hszg.de/thermo_fpc/)

[b]values for water calculated according to the IAPWS recommendations (http://www.iapws.org/relguide/dielec.pdf)

Table S4. The value of molar concentration of salt C_{salt} [mol/dm^3], concentration of CD C_{Cd} [mol/dm^3], molar conductivity Λ [S·cm^2·mol^{-1}] for α-cyclodextrin (α-CD) with dacarbazine (DTIC) in water at all tested temperatures at pressure p = 0.1 MPa.[a]

			α-cyclodextrin (α-CD)				
T [K]			283.15	298.15	303.15	308.15	313.15
Nr	c_{salt} [mol/dm^3]	C_{Cd} [mol/dm^3]	Λ_m [S·cm^2·mol^{-1}]	Λ_m [S·cm^2·mol^{-1}]	Λ_m [S·cm^2·mol^{-1}]	Λ_m S·cm^2·mol^{-1}]	Λ_m S·cm^2·mol^{-1}]
1.	0.00336	0.00000	58.6371	65.4451	70.4551	79.7197	85.7585
2.	0.00332	0.00024	58.0358	64.3139	69.3139	78.3494	84.9254
3.	0.00330	0.00034	57.7261	63.0466	68.0466	77.2996	84.3408
4.	0.00327	0.00048	57.3521	61.8202	66.8202	76.3779	83.6545
5.	0.00325	0.00061	56.9879	60.5763	65.5763	75.3714	82.8807
6.	0.00321	0.00078	56.5004	59.3339	64.3339	73.8916	82.1244
7.	0.00318	0.00092	56.1098	58.1578	63.1588	72.3621	81.3432
8.	0.00315	0.00107	55.6821	57.0393	62.0393	70.9685	80.6511
9.	0.00312	0.00122	55.1642	56.1847	61.1847	69.7074	79.9165
10	0.00308	0.00143	54.6724	55.6365	60.6365	68.7348	78.9239
11	0.00304	0.00163	54.0607	55.3173	60.3173	68.0572	77.8810
12	0.00300	0.00184	53.4228	55.1134	60.1134	67.6576	76.9524
13	0.00297	0.00201	52.9162	54.9841	59.9841	67.4632	75.9657
14	0.00293	0.00223	52.3630	54.8750	59.8750	67.2821	74.9964
15	0.00287	0.00251	51.7675	54.7947	59.7947	67.1296	74.0091
16	0.00281	0.00280	51.3344	54.7369	59.7369	67.0207	73.1524
17	0.00275	0.00311	51.0885	54.6984	59.6984	66.9516	72.6355
18	0.00269	0.00341	50.9508	54.6264	59.6264	66.8760	72.2723
19	0.00264	0.00368	50.8979	54.5517	59.5517	66.8308	72.1069
20	0.00258	0.00398	50.8093	54.5414	59.5414	66.7371	71.9432
21	0.00251	0.00431	50.8033	54.4920	59.4920	66.7140	71.7653
22	0.00245	0.00462	50.7557	54.4535	59.4635	66.6466	71.6055
23	0.00239	0.00491	50.7283	54.4237	59.4237	66.6352	71.4917
24	0.00233	0.00522	50.6857	54.3892	59.3892	66.5354	71.2195
25	0.00227	0.00550	50.6484	54.3223	59.3623	66.4586	71.1472
26	0.00221	0.00578	50.6012	54.3123	59.3023	66.3054	70.9917
27	0.00217	0.00608	50.5936	54.2541	59.2533	66.2723	70.9087
28	0.00210	0.00638	50.5815	54.2024	59.2124	66.1932	70.7597

[a] Standard uncertainties are $u(T) = 0.01$ K, $u(p) = 0.05$ MPa, $u(c) = 10^{-4} \cdot c$, and the combined expanded uncertainty is $U_c(\Lambda) = 0.0005 \cdot \Lambda$ (level of confidence = 0.95).

Table S5. The value of molar concentration of salt C_{salt} [mol/dm^3], concentration of CD C_{Cd} [mol/dm^3], molar conductivity Λ [S·cm^2·mol^{-1}] for hydroxypropyl-β-cyclodextrin (HP-β-CD) with dacarbazine (DTIC) in water at all tested temperatures at pressure p = 0.1 MPa.[a]

hydroxypropyl-β-cyclodextrin (HP-β-CD)							
T [K]			283.15	298.15	303.15	308.15	313.15
Nr	c_{salt} mol/dm^3]	C_{Cd} [mol/dm^3]	Λ_m [S·cm^2·mol^{-1}]	Λ_m [S·cm^2·mol^{-1}]	Λ_m [S·cm^2·mol^{-1}]	Λ_m S·cm^2·mol^{-1}]	Λ_m S·cm^2·mol^{-1}]
1.	0.00304	0.00000	64.7252	67.5068	72.7309	82.0947	88.0679
2.	0.00301	0.00026	63.9428	66.3555	71.5796	81.1891	86.6698
3.	0.00299	0.00039	63.4142	65.7218	70.9460	80.5376	85.9741
4.	0.00297	0.00058	62.8972	64.8200	70.0442	79.6505	85.2783
5.	0.00296	0.00067	62.3811	64.2355	69.4596	79.2274	84.3041
6.	0.00294	0.00080	61.8538	63.3726	68.5967	78.6690	83.4709
7.	0.00292	0.00094	61.2259	62.8278	68.0519	78.0361	82.5384
8.	0.00290	0.00108	60.6871	62.0017	67.2258	77.3293	81.9537
9.	0.00289	0.00119	60.1615	61.2968	66.5209	76.7920	80.9923
10	0.00285	0.00147	59.3895	60.2829	65.5070	75.3943	79.8545
11	0.00283	0.00169	58.6626	59.3302	64.5544	74.3259	78.8135
12	0.00280	0.00190	57.9480	58.4615	63.6856	73.3497	77.5867
13	0.00277	0.00210	57.2476	57.6813	62.9054	72.4974	76.4282
14	0.00274	0.00237	56.5913	57.0319	62.2560	71.3975	75.5683
15	0.00269	0.00273	55.8084	56.2858	61.5099	70.2155	74.2275
16	0.00266	0.00299	55.1194	55.7450	60.9691	69.5657	73.0799
17	0.00261	0.00335	54.6044	55.3292	60.5533	68.9600	72.2722
18	0.00258	0.00361	54.2090	55.0443	60.2685	68.6863	71.7202
19	0.00254	0.00393	53.8408	54.8304	60.0545	68.4101	71.1600
20	0.00250	0.00423	53.5442	54.6413	59.8654	68.2121	70.9371
21	0.00246	0.00454	53.4012	54.4890	59.7131	68.0479	70.6896
22	0.00242	0.00482	53.1831	54.3471	59.5712	67.9302	70.4649
23	0.00238	0.00512	52.9968	54.2181	59.4422	67.8199	70.2833
24	0.00235	0.00539	52.7911	54.1024	59.3265	67.7111	70.0309
25	0.00231	0.00570	52.6260	53.9617	59.1859	67.6226	69.8413
26	0.00226	0.00608	52.3958	53.9405	59.1647	67.5317	69.5544
27	0.00184	0.00629	52.3047	53.8476	59.0718	67.5663	69.5246
28	0.00178	0.00642	52.2985	53.8112	58.9981	67.5562	69.4824

Table S6. The value of molar concentration of salt C_{salt} [mol/dm^3], concentration of CD C_{Cd} [mol/dm^3], molar conductivity Λ [S·cm^2·mol^{-1}] for hydroxyethyl-β-cyclodextrin (HE-β-CD) with dacarbazine (DTIC) in water at all tested temperatures at pressure p = 0.1 MPa.[a]

hydroxyethyl-β-cyclodextrin (HE-β-CD)							
T [K]			283.15	298.15	303.15	308.15	313.15
Nr	c_{salt} [mol/dm^3]	C_{Cd} [mol/dm^3]	Λ_m [S·cm^2·mol^{-1}]	Λ_m [S·cm^2·mol^{-1}]	Λ_m [S·cm^2·mol^{-1}]	Λ_m S·cm^2·mol^{-1}]	Λ_m S·cm^2·mol^{-1}]
1.	0.00296	0.00000	60.9992	67.7315	72.8980	82.0997	87.9826
2.	0.00292	0.00026	60.4878	67.2201	72.3865	81.5882	87.4711
3.	0.00290	0.00033	60.3117	67.0440	72.2104	81.4122	87.2950
4.	0.00287	0.00047	59.9661	66.6984	71.8648	81.0665	86.9494
5.	0.00285	0.00062	59.6837	66.4160	71.5824	80.7842	86.6670
6.	0.00282	0.00076	59.2792	66.0115	71.1779	80.3796	86.2625
7.	0.00279	0.00091	59.0077	65.7400	70.9064	80.1081	85.9910

8.	0.00276	0.00108	58.6647	65.3970	70.5634	79.7651	85.6480
9.	0.00274	0.00121	58.3361	65.0684	70.2348	79.4366	85.3194
10	0.00270	0.00142	57.8199	64.5522	69.7186	78.9203	84.8032
11	0.00266	0.00163	57.4755	64.2078	69.3742	78.5759	84.4588
12	0.00262	0.00183	57.0926	63.8249	68.9913	78.1930	84.0759
13	0.00258	0.00204	56.6983	63.4306	68.5970	77.7988	83.6816
14	0.00257	0.00221	56.3731	63.1054	68.2718	77.4736	83.3564
15	0.00249	0.00251	56.0833	62.8156	67.9820	77.1837	83.0666
16	0.00244	0.00280	55.8699	62.6022	67.7686	76.9704	82.8532
17	0.00238	0.00309	55.7407	62.4730	67.6394	76.8411	82.7240
18	0.00233	0.00339	55.6786	62.4109	67.5773	76.7790	82.6619
19	0.00227	0.00372	55.7370	62.4693	67.6357	76.8374	82.7203
20	0.00222	0.00398	55.7213	62.4536	67.6200	76.8218	82.7046
21	0.00216	0.00428	55.6937	62.4260	67.5924	76.7941	82.6770
22	0.00211	0.00457	55.7175	62.4498	67.6162	76.8179	82.7008
23	0.00206	0.00484	55.6751	62.4074	67.5738	76.7755	82.6584
24	0.00199	0.00518	55.7128	62.4451	67.6115	76.8132	82.6961
25	0.00194	0.00546	55.7138	62.4461	67.6125	76.8142	82.6971
26	0.00188	0.00576	55.7197	62.4520	67.6184	76.8201	82.7030
27	0.00183	0.00604	55.6691	62.4014	67.5678	76.7695	82.6524
28	0.00179	0.00625	55.6433	62.3756	67.5620	76.7537	82.6266

Table 7. ΔS [kJ/mol·K] in the temperature range 293.15–313.15 K calculated for the α-CD:DTIC, HP-β-CD:DTIC and HE-β-CD:DTIC complexes presented in Figure 4 of the main article. Experimental values (EXP) are written in blue.

α-CD:DTIC	**ΔS PCM**	**ΔS CPCM**	**ΔS SMD**	**ΔS Onsag**	**ΔS EXP**
293.15					
K02_03	**-0.25**	**-0.25**	**-0.26**	**-0.25**	**-0.2506**
K01_01	-0.26	-0.26	-0.26	-0.26	
K03_03	-0.26	-0.26	-0.25	-0.25	
298.15					
K02_03	-0.25	-0.25	-0.26	-0.25	**-0.2502**
K01_01	-0.26	-0.26	-0.26	-0.26	
K03_03	-0.26	-0.25	-0.25	-0.25	
303.15					
K02_03	-0.25	-0.25	-0.26	-0.25	**-0.2594**
K01_01	-0.26	-0.22	-0.26	-0.26	
K03_03	-0.26	-0.25	-0.25	-0.25	
308.15					
K02_03	-0.25	-0.25	-0.26	-0.25	**-0.3123**
K01_01	-0.26	-0.26	-0.26	-0.27	
K03_03	-0.26	-0.25	-0.25	-0.25	
313.15					
K02_03	-0.25	-0.25	-0.26	-0.25	**-0.3417**
K01_01	-0.26	-0.27	-0.26	-0.26	
K03_03	**-0.25**	**-0.25**	**-0.25**	**-0.25**	
HP-β-CD:DTIC	**ΔS PCM**	**ΔS CPCM**	**ΔS SMD**	**ΔS Onsag**	**ΔS EXP**
293.15					

K03_03	-0.27	-0.27	-0.29	-0.26	**-0.29**
K04_03	-0.26	-0.26	-0.28	-0.26	
K04_01	-0.27	-0.27	-0.30	-0.29	
298.15					
K03_03	-0.27	-0.27	-0.29	-0.26	**-0.31**
K04_03	-0.26	-0.26	-0.28	-0.26	
K04_01	-0.27	-0.27	-0.30	-0.29	
303.15					
K03_03	-0.27	-0.27	-0.29	-0.25	**-0.33**
K04_03	-0.26	-0.26	-0.28	-0.25	
K04_01	-0.27	-0.27	-0.30	-0.27	
308.15					
K03_03	-0.27	-0.27	-0.29	-0.26	**-0.35**
K04_03	-0.26	-0.26	-0.28	-0.26	
K04_01	-0.27	-0.27	-0.28	-0.26	
313.15					
K03_03	-0.27	-0.27	-0.29	-0.26	**-0.37**
K04_03	-0.26	-0.26	-0.28	-0.26	
K04_01	**-0.27**	**-0.27**	**-0.30**	**-0.29**	
HE-β-CD:DTIC	**ΔS PCM**	**ΔS CPCM**	**ΔS SMD**	**ΔS Onsag**	**ΔS EXP**
293.15					
K04_01	-0.32	-0.32	-0.33	-0.32	**-0.48**
K03_02	-0.30	-0.30	-0.32	-0.31	
K03_03	-0.30	-0.30	-0.32	-0.30	
298.15					
K04_01	-0.32	-0.32	-0.33	-0.32	**-0.46**
K03_02	-0.30	-0.30	-0.32	-0.31	
K03_03	-0.30	-0.30	-0.32	-0.30	
303.15					
K04_01	-0.32	-0.32	-0.33	-0.32	**-0.40**
K03_02	-0.30	-0.30	-0.32	-0.31	
K03_03	-0.30	-0.30	-0.32	-0.30	
308.15					
K04_01	-0.32	-0.32	-0.33	-0.31	**-0.38**
K03_02	-0.30	-0.30	-0.32	-0.31	
K03_03	-0.30	-0.30	-0.32	-0.30	
313.15					
K04_01	-0.32	-0.32	-0.33	-0.30	**-0.35**
K03_02	-0.30	-0.30	-0.32	-0.31	
K03_03	-0.30	-0.30	-0.32	-0.30	

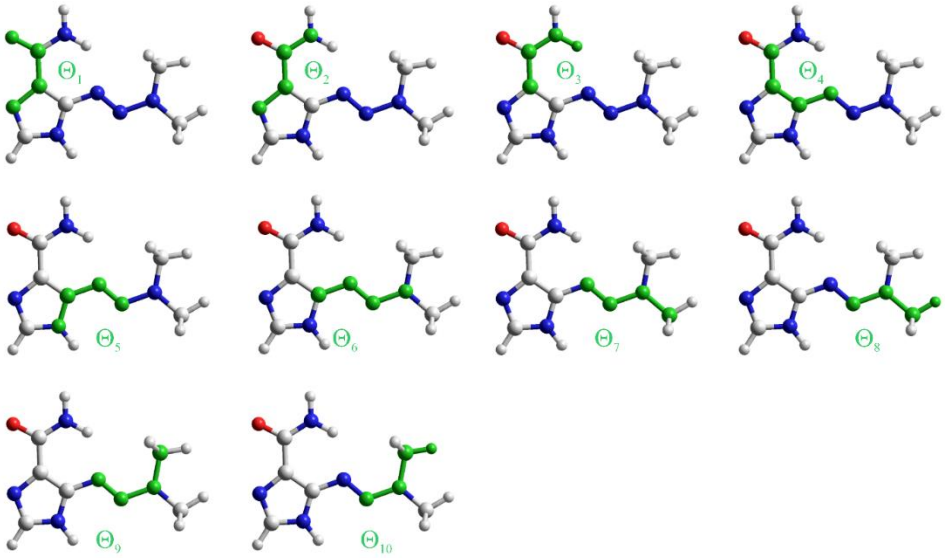


Figure S6. Torsion angles (θ; green highlight) marked in dacarbazine and changed during the conformational procedure performed in HyperChem.