Supplementary Information: Spontaneous generation of hydrogen from water using modified dodecaborate ions

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Number of pages: 122

Number of figures: 6

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SI   Benchmark for the level of theory

We employed the B3LYP hybrid functional in combination with the Stuttgart/Dresden effective core potential for iodine and the 6-31+G(d,p) basis set for the remaining atoms, as this approach has previously performed in good agreement with experiment. However, we tested different levels of theory to determine whether there was an impact on energetic

terms. For this test, we chose the hydrogen-generation step for $[B_{12}Br_{10}]^{-\bullet}$ and $[B_{12}I_{10}]^{-\bullet}$. For $[B_{12}Br_{10}]^{-\bullet}$, we tested both the B3LYP/aug-cc-pVTZ and B3LYP-D3BJ/aug-cc-pVTZ levels on all the types of atoms. For $[B_{12}I_{10}]^{-\bullet}$, we tried the B3LYP/SDD//aug-cc-pVTZ and B3LYP-D3BJ/SDD//aug-cc-pVTZ with the SDD effective core potential only applied to the iodine atoms. The results, including the values reported in the main text for comparison, are contained in the following tables.

Table S1: Relative energies (in eV) for different levels of theory for the hydrogen generation step in Figure 4 of the main text.

Level of theory	$[B_{12}Br_{10}(H_2O)_2]^-$	TS1	$[B_{12}Br_{10}(OH)_2]^- + H_2$
"B3LYP/6-31+G(d,p)"	0	0.06	-2.38
B3LYP/aug-cc-pVTZ	0	0.12	-2.26
B3LYP-D3BJ/aug-cc-pVTZ	0	0.09	-2.15

Table S2: Relative energies (in eV) for different levels of theory for the hydrogen generation step in Figure 5 of the main text.

Level of theory	$[B_{12}I_{10}(H_2O)_2]^-$	TS5	$[B_{12}I_{10}(OH)_2]^- + H_2$
"B3LYP/SDD//6-31+G(d,p)"	0	-0.13	-2.05
B3LYP/SDD//aug-cc-pVTZ	0	-0.03	-2.02
B3LYP-D3BJ/SDD//aug-cc-pVTZ	0	-0.12	-1.95

As shown in the results, the energetics follow the same trend, and we don't expect that, including the tested higher levels of theory, will dramatically affect the main results of our study. Accordingly, we proceeded with our studies employing the B3LYP hybrid functional together with the Stuttgart/Dresden effective core potential for iodine and the 6-31+G(d,p) basis set for all other atoms.

SII Optimized geometries, Hirshfeld charges, and condensed Fukui functions

SII.1 Optimized geometries

Table S3: Optimized geometries in Å for species of the $[B_{12}X_{12}]^{2-}$ type (X = Br, I, CN).

	$[B_{12}Br_{12}]^{2-}$			$[B_{12}I_{12}]^{2-}$				$[B_{12}(CN)_{12}]^{2-}$		
Atom	x	y	z	x	y	z	Atom	x	y	z
1B	1.2786	-0.4492	1.0328	0.8089	0.6281	1.3707	1B	1.6818	-0.2838	-0.1143
2B	1.4964	-0.3366	-0.7421	1.2519	1.1266	-0.3	2B	0.5562	-1.5251	0.5368
3B	0.4775	-1.635	-0.0452	1.6	-0.5464	0.2613	3B	0.8734	-0.0216	1.4698
4B	-0.4111	-0.9515	1.3523	0.2368	-1.0763	1.3086	4B	1.0231	1.3366	0.3010
5B	0.0587	0.7693	1.5192	-0.9539	0.2694	1.3945	5B	0.7982	0.6719	-1.3545
6B	1.2377	1.1493	0.2249	-0.3264	1.6309	0.4004	6B	0.5098	-1.0967	-1.2086
7B	-0.0587	-0.7693	-1.5192	0.9537	-0.2694	-1.3944	7B	-0.7985	-0.6718	1.3546
8B	-1.2377	-1.1493	-0.2249	0.3266	-1.6308	-0.4001	8B	-0.5099	1.0967	1.2087
9B	-1.4964	0.3366	0.7421	-1.2517	-1.1266	0.3	9B	-0.5564	1.5252	-0.5366
10B	-0.4775	1.635	0.0451	-1.5998	0.5464	-0.2612	10B	-0.8737	0.0215	-1.4697
11B	0.4111	0.9515	-1.3523	-0.2367	1.0764	-1.3083	11B	-1.0234	-1.3364	-0.3008
12B	-1.2786	0.4492	-1.0328	-0.8087	-0.628	-1.3705	12B	-1.6830	0.2841	0.1146
13X	1.0285	-3.5221	-0.0975	1.8567	1.4417	3.1461	13C	1.0588	-2.9016	1.0211
14X	-0.8856	-2.0499	2.913	2.8741	2.5868	-0.6889	14C	1.6627	-0.0405	2.7959
15X	0.1265	1.6572	3.2727	3.6734	-1.2545	0.5996	15C	1.9473	2.5425	0.5721
16X	2.6662	2.4758	0.4842	0.544	-2.4709	3.0039	16C	1.5199	1.2782	-2.5765
17X	-0.1265	-1.6573	-3.2727	-2.1892	0.6185	3.2012	17C	0.9706	-2.0863	-2.2996
18X	-2.6662	-2.4758	-0.4842	-0.7491	3.7442	0.9189	18C	-1.5197	-1.2785	2.5768
19X	-3.2237	0.725	1.5983	2.1896	-0.6185	-3.2014	19C	-0.9703	2.0864	2.2998
20X	-1.0285	3.5221	0.0975	0.749	-3.7443	-0.9194	20C	-1.0587	2.9016	-1.0216
21X	0.8856	2.0499	-2.9131	-2.8741	-2.5867	0.6895	21C	-1.6627	0.0406	-2.7960
22X	-2.7546	0.968	-2.2243	-3.6734	1.2548	-0.5992	22C	-1.9470	-2.5426	-0.5724
23X	2.7546	-0.9679	2.2244	-0.5441	2.4706	-3.0043	23C	-3.2012	0.5406	0.2181
24X	3.2237	-0.725	-1.5983	-1.857	-1.4418	-3.1461	24N	-2.2571	0.0546	-3.7954
							25N	1.4375	-3.9387	1.3862
							26N	2.6437	3.4512	0.7760
							27N	2.2577	-0.0543	3.7950
							28N	1.3178	-2.8319	-3.1216
							29N	2.0637	1.7350	-3.4974
							30N	-1.4371	3.9386	-1.3872
							31N	-2.6429	-3.4516	-0.7769
							32N	-4.3453	0.7338	0.2960
							33N	-1.3169	2.8325	3.1217
							34N	-2.0630	-1.7358	3.4977
							35C	3.1999	-0.5404	-0.2176
							36N	4.3440	-0.7339	-0.2949

Table S4: Optimized geometries in Å for species of the $[B_{12}Br_{11}]^q$ type (q = 2-, 1-, 0).

	$[B_{12}Br_{11}]^{2-}$			$[B_{12}Br_{11}]^-$			$B_{12}Br_{11}$		
Atom	x	y	z	x	y	z	x	y	z
1B	0	0	-1.9032	-0.0002	0.0001	-1.6989	-0.0017	-0.0144	-1.7062
2B	0.0082	-1.5189	-1.0408	-0.2895	-1.5317	-0.9951	0.1716	1.5405	-1.0414
3B	1.447	-0.4615	-1.0409	1.3676	-0.7487	-0.9947	-1.4491	0.6002	-1.0056
4B	0.886	1.2336	-1.0409	1.1347	1.0693	-0.9947	-1.0393	-1.1853	-0.9959
5B	-0.8994	1.2239	-1.0409	-0.6665	1.4097	-0.9945	0.7599	-1.3803	-0.997
6B	-1.4419	-0.4773	-1.0409	-1.5468	-0.198	-0.9943	1.5451	0.2731	-1.0042
7B	0.9059	-1.2326	0.4841	0.6573	-1.3906	0.5233	-0.7495	1.3571	0.5187
8B	1.4522	0.4807	0.4841	1.5259	0.1955	0.5233	-1.5234	-0.2873	0.5296
9B	-0.0084	1.5297	0.4841	0.2857	1.5115	0.5234	-0.168	-1.5179	0.5714
10B	-1.4573	0.4647	0.4841	-1.3493	0.7388	0.5236	1.4241	-0.6097	0.5316
11B	-0.8923	-1.2425	0.4842	-1.1195	-1.0549	0.5236	1.0244	1.1648	0.5174
12B	0	0	1.4216	0.0001	0	1.4505	0.0013	0.0102	1.4634
13Br	3.1195	-0.9948	-1.9595	2.8385	-1.5537	-1.9876	-2.9648	1.2813	-1.9831
14Br	1.9101	2.6594	-1.9595	2.355	2.2192	-1.9878	-2.1616	-2.4371	-1.9431
15Br	-1.9392	2.6382	-1.9596	-1.3831	2.9257	-1.9875	1.5849	-2.8451	-1.9432
16Br	-3.1086	-1.0289	-1.9593	-3.2101	-0.4107	-1.9872	3.1742	0.6093	-1.9803
17Br	1.9462	-2.6479	1.3746	1.4054	-2.9731	1.3808	-1.6072	2.881	1.3329
18Br	3.1198	1.0326	1.3743	3.2619	0.4176	1.3813	-3.2209	-0.6232	1.3795
19Br	-0.018	3.2862	1.3745	0.6107	3.2313	1.3813	-0.3547	-3.2266	1.4362
20Br	-3.1308	0.9984	1.3745	-2.8844	1.579	1.3818	3.0076	-1.3052	1.3822
21Br	-1.917	-2.6691	1.3746	-2.3929	-2.2556	1.3813	2.1908	2.4671	1.3335
22Br	0.0001	0.0001	3.3915	0.0003	-0.0003	3.4038	0.0038	0.0344	3.4019
23Br	0.018	-3.2743	-1.9595	-0.6013	-3.1797	-1.9881	0.3485	3.1711	-2.0423

Table S5: Optimized geometries in Å for species of the $[B_{12}I_{11}]^q$ type (q = 2-, 1-, 0).

	$[B_{12}I_{11}]^{2-}$			$[B_{12}I_{11}]^{-}$			$B_{12}I_{11}$		
Atom	x	y	z	x	y	z	x	y	z
1B	0	0	-1.9024	0.0001	-0.0002	-1.6986	0	-0.0001	-1.7143
2B	-1.3585	-0.6868	-1.0509	-1.3465	-0.7898	-1.0025	-1.3745	-0.7302	-1.0138
3B	0.2333	-1.5042	-1.0509	0.335	-1.5247	-1.0025	0.2697	-1.533	-1.0136
4B	1.5028	-0.2429	-1.051	1.5537	-0.1525	-1.0025	1.5412	-0.2172	-1.0137
5B	0.6955	1.3541	-1.051	0.6251	1.4304	-1.0027	0.6828	1.3986	-1.0138
6B	-1.073	1.0799	-1.051	-1.1674	1.0366	-1.0025	-1.1192	1.0816	-1.0139
7B	-0.7024	-1.3678	0.4781	-0.6188	-1.4162	0.52	-0.6727	-1.3781	0.5064
8B	1.0838	-1.0906	0.478	1.1558	-1.0263	0.5201	1.1027	-1.0656	0.5064
9B	1.3721	0.6938	0.4781	1.3332	0.782	0.5199	1.3541	0.7195	0.5063
10B	-0.2358	1.5193	0.4779	-0.3318	1.5097	0.52	-0.2658	1.5104	0.5063
11B	-1.5178	0.2454	0.478	-1.5383	0.151	0.5201	-1.5185	0.214	0.5062
12B	0	0	1.4173	0	0.0001	1.4521	0	0	1.4484
13I	-3.1045	-1.5694	-2.124	-2.9608	-1.7371	-2.1463	-3.0282	-1.6089	-2.1385
14I	0.5333	-3.4375	-2.1239	0.737	-3.3527	-2.1465	0.5944	-3.3771	-2.1385
15I	3.4342	-0.5552	-2.1239	3.4165	-0.3352	-2.1463	3.3954	-0.4783	-2.1387
16I	1.5894	3.0945	-2.1238	1.3744	3.1456	-2.1465	1.5041	3.0813	-2.1389
17I	-2.4519	2.4677	-2.124	-2.5672	2.2792	-2.1463	-2.4659	2.3828	-2.1387
18I	-1.6107	-3.1366	1.4601	-1.4122	-3.2321	1.4663	-1.5374	-3.1494	1.464
19I	2.4853	-2.5011	1.4601	2.6375	-2.342	1.4665	2.5203	-2.4353	1.464
20I	3.1466	1.5908	1.4602	3.0424	1.7848	1.4661	3.095	1.6443	1.4638
21I	-0.5406	3.4842	1.46	-0.7572	3.4451	1.4662	-0.6074	3.4517	1.464
22I	-3.4808	0.5627	1.46	-3.5105	0.3442	1.4663	-3.4703	0.4889	1.4639
23I	-0.0001	-0.0001	3.635	0	0.0002	3.6512	0	0.0001	3.638

Table S6: Optimized geometries in Å for species of the $[B_{12}(CN)_{11}]^q$ type (q = 2-, 1-, 0).

	$[B_{12}(CN)_{11}]^{2-}$			$[B_{12}(CN)_{11}]^-$			$B_{12}(CN)_{11}$		
Atom	x	y	z	x	y	z	x	y	z
1B	0.0002	0.0001	-1.9051	0.0002	-0.0003	-1.657	-0.008	0	-1.6742
2B	0.2496	-1.5042	-1.011	-1.0538	1.1633	-0.9677	1.282	0.9126	-0.9933
3B	1.5079	-0.2275	-1.0107	-1.4321	-0.6432	-0.9674	-0.4582	1.5138	-0.9768
4B	0.6825	1.3637	-1.0108	0.169	-1.5608	-0.9672	-1.5732	-0.0004	-0.9932
5B	-1.0859	1.0705	-1.0109	1.5368	-0.3219	-0.967	-0.4573	-1.5141	-0.9768
6B	-1.3535	-0.702	-1.0111	0.7808	1.3618	-0.9676	1.2826	-0.9118	-0.9933
7B	1.0909	-1.0752	0.5258	-1.511	0.3163	0.5608	0.4604	1.485	0.5557
8B	1.3596	0.7053	0.526	-0.7678	-1.3393	0.5612	-1.2642	0.8958	0.5673
9B	-0.2507	1.511	0.5259	1.0364	-1.1442	0.5614	-1.2637	-0.8965	0.5673
10B	-1.5146	0.2286	0.5257	1.4084	0.6321	0.5611	0.4613	-1.4848	0.5557
11B	-0.6855	-1.3698	0.5257	-0.1661	1.5346	0.561	1.5377	0.0005	0.5774
12B	-0.0001	-0.0001	1.4666	-0.0001	0	1.4877	0.0081	0	1.4951
13C	0.4752	-2.8645	-1.713	-1.9428	2.1446	-1.74	2.3606	1.6922	-1.7344
14C	2.8715	-0.4332	-1.7125	-2.6401	-1.1854	-1.7397	-0.8856	2.7638	-1.7334
15C	1.2997	2.5968	-1.7127	0.3113	-2.8768	-1.7402	-2.8899	-0.0009	-1.7495
16C	-2.068	2.0386	-1.7128	2.833	-0.5934	-1.7391	-0.884	-2.7643	-1.7334
17C	-2.5775	-1.337	-1.7131	1.4398	2.5104	-1.7396	2.3616	-1.6908	-1.7344
18C	2.0734	-2.0438	1.2193	-2.8617	0.5993	1.2345	0.8874	2.7838	1.228
19C	2.5842	1.3405	1.2197	-1.4542	-2.5361	1.2355	-2.3757	1.7071	1.2241
20C	-0.4764	2.872	1.2196	1.9625	-2.1667	1.236	-2.3747	-1.7085	1.2241
21C	-2.8788	0.4345	1.2191	2.6671	1.1973	1.2351	0.889	-2.7832	1.228
22C	-1.303	-2.6036	1.2191	-0.3144	2.9063	1.2351	2.9065	0.0008	1.2414
23C	-0.0003	-0.0003	3.0111	-0.0004	0.0006	3.0252	0.0073	0	3.0249
24N	-3.9092	0.59	1.7359	3.6241	1.6267	1.7361	1.2197	-3.7794	1.7356
25N	0.6434	-3.8797	-2.2554	-2.6086	2.8797	-2.3459	3.178	2.2846	-2.3135
26N	1.7602	3.5171	-2.255	0.4182	-3.8627	-2.3464	-3.8938	-0.0011	-2.3415
27N	3.8891	-0.5867	-2.2548	-3.5453	-1.5912	-2.3453	-1.2111	3.7125	-2.3245
28N	-3.4912	-1.8107	-2.2554	1.9332	3.3706	-2.3458	3.1792	-2.283	-2.3134
29N	-2.8007	2.7612	-2.255	3.8037	-0.797	-2.3449	-1.2091	-3.7132	-2.3245
30N	-0.6468	3.8998	1.7367	2.6664	-2.9441	1.7374	-3.2282	-2.3304	1.7164
31N	-1.7693	-3.5354	1.7358	-0.4269	3.9492	1.7361	3.9595	0.0011	1.7443
32N	-0.0003	-0.0006	4.174	-0.0007	0.0011	4.1873	0.0101	0.0001	4.1883
33N	3.5091	1.8201	1.7367	-1.9761	-3.4456	1.7371	-3.2295	2.3287	1.7164
34N	2.8154	-2.7755	1.7358	-3.8883	0.8146	1.7353	1.2177	3.7801	1.7354

Table S7: Optimized geometries in Å for species of the $[B_{12}Br_{10}]^q$ type (q = 2-, 1-, 0).

	$[B_{12}Br_{10}]^{2-}$			$[B_{12}Br_{10}]^{-}$			$B_{12}Br_{10}$		
Atom	x	y	z	x	y	z	x	y	z
1B	0	-0.7873	-1.8525	0	-0.8077	-1.7888	0	-0.8387	-1.6959
2B	0	0.7873	-1.8525	0	0.8077	-1.7888	0	0.8387	-1.6959
3B	-1.4489	0	-1.3998	-1.4711	0	-1.3746	-1.4699	0	-1.3678
4B	-0.908	-1.4584	-0.5338	-0.9172	-1.4698	-0.4821	-0.9257	-1.495	-0.4347
5B	0.908	-1.4584	-0.5338	0.9172	-1.4698	-0.4821	0.9257	-1.495	-0.4347
6B	1.4489	0	-1.3998	1.4711	0	-1.3746	1.4699	0	-1.3678
7B	-0.908	1.4583	-0.5338	-0.9172	1.4698	-0.4821	-0.9257	1.495	-0.4347
8B	-1.4743	0	0.3792	-1.4746	0	0.4141	-1.4732	0	0.4407
9B	0	-0.8965	0.9108	0	-0.8975	0.9555	0	-0.9048	0.9989
10B	1.4743	0	0.3792	1.4746	0	0.4141	1.4732	0	0.4407
11B	0.908	1.4584	-0.5338	0.9172	1.4698	-0.4821	0.9257	1.495	-0.4347
12B	0	0.8965	0.9108	0	0.8975	0.9555	0	0.9048	0.9989
13Br	-3.1228	0	-2.5183	-3.0459	0	-2.5516	-2.956	0	-2.6192
14Br	-1.9392	-3.1549	-0.5439	-1.9322	-3.1382	-0.5477	-1.9464	-3.134	-0.5216
15Br	1.9392	-3.1549	-0.5439	1.9322	-3.1382	-0.5477	1.9464	-3.1341	-0.5216
16Br	3.1228	0	-2.5183	3.0459	0	-2.5516	2.9559	0	-2.6193
17Br	-1.9392	3.1549	-0.5439	-1.9322	3.1382	-0.5477	-1.9464	3.1341	-0.5216
18Br	-3.1321	0	1.4461	-3.14	0	1.428	-3.1632	0	1.3807
19Br	0	-1.925	2.5929	0	-1.9296	2.6131	0	-1.929	2.6379
20Br	3.1321	0	1.4461	3.14	0	1.428	3.1632	0	1.3807
21Br	1.9392	3.1549	-0.5439	1.9322	3.1382	-0.5477	1.9464	3.134	-0.5216
22Br	0	1.925	2.5929	0	1.9296	2.6131	0	1.929	2.6379

Table S8: Optimized geometries in Å for species of the $[B_{12}I_{10}]^q$ type (q = 2-, 1-, 0).

	$[B_{12}I_{10}]^{2-}$			$[B_{12}I_{10}]^{-}$			$B_{12}I_{10}$		
Atom	x	y	z	x	y	z	x	y	z
1B	0	-0.7868	-1.862	0	-0.8067	-1.7949	0	-0.8318	-1.6932
2B	0	0.7868	-1.862	0	0.8066	-1.7949	0	0.8318	-1.6932
3B	-1.4516	0	-1.4287	-1.4685	0	-1.3933	-1.4616	0	-1.3593
4B	-0.9129	-1.4631	-0.5574	-0.9212	-1.473	-0.4978	-0.9272	-1.4876	-0.4298
5B	0.9129	-1.4631	-0.5574	0.9212	-1.473	-0.4978	0.9272	-1.4876	-0.4298
6B	1.4516	0	-1.4287	1.4685	0	-1.3933	1.4616	0	-1.3593
7B	-0.9129	1.4631	-0.5574	-0.9212	1.473	-0.4978	-0.9272	1.4876	-0.4298
8B	-1.4837	0	0.3576	-1.485	0	0.401	-1.4858	0	0.4493
9B	0	-0.902	0.891	0	-0.9022	0.9438	0	-0.9052	1.0082
10B	1.4837	0	0.3576	1.485	0	0.401	1.4858	0	0.4493
11B	0.9129	1.4631	-0.5574	0.9212	1.473	-0.4978	0.9272	1.4876	-0.4298
12B	0	0.902	0.891	0	0.9022	0.9438	0	0.9052	1.0082
13I	-3.2988	0	-2.7499	-3.1748	0	-2.8006	-3.0219	0	-2.8912
14I	-2.0616	-3.3773	-0.6295	-2.0511	-3.3536	-0.6298	-2.0534	-3.3429	-0.6104
15I	2.0616	-3.3773	-0.6295	2.0511	-3.3536	-0.6298	2.0534	-3.3429	-0.6104
16I	3.2988	0	-2.7499	3.1748	0	-2.8006	3.0219	0	-2.8912
17I	-2.0616	3.3773	-0.6295	-2.0511	3.3536	-0.6298	-2.0534	3.3429	-0.6104
18I	-3.3646	0	1.5355	-3.369	0	1.5269	-3.3936	0	1.5019
19I	0	-2.075	2.7712	0	-2.0773	2.8012	0	-2.0843	2.8418
20I	3.3646	0	1.5355	3.369	0	1.5269	3.3936	0	1.5019
21I	2.0616	3.3773	-0.6295	2.0511	3.3536	-0.6298	2.0534	3.3429	-0.6104
22I	0	2.075	2.7712	0	2.0773	2.8012	0	2.0843	2.8418

Table S9: Optimized geometries in Å for species of the $[B_{12}(CN)_{10}]^q$ type (q = 2-, 1-, 0).

	$[B_{12}(CN)_{10}]^{2-}$			$[B_{12}(CN)_{10}]^{-}$			$B_{12}(CN)_{10}$		
Atom	x	y	z	x	y	z	x	y	z
1B	0.0001	0.7847	-1.8136	0	0.8063	-1.7337	0	0.8449	-1.6474
2B	0	-0.7844	-1.8136	0	-0.8071	-1.7339	0	-0.8465	-1.6469
3B	1.4635	0	-1.3239	1.4881	-0.0002	-1.309	1.4893	-0.0008	-1.33
4B	0.909	1.4656	-0.4641	0.9214	1.4772	-0.4164	0.9328	1.5109	-0.3858
5B	-0.9088	1.4657	-0.4641	-0.9214	1.4773	-0.4164	-0.9328	1.5109	-0.3858
6B	-1.4633	0.0002	-1.324	-1.4881	-0.0001	-1.309	-1.4893	-0.0007	-1.33
7B	0.9088	-1.4659	-0.4646	0.9215	-1.4777	-0.4164	0.933	-1.5111	-0.3844
8B	1.4733	-0.0001	0.4683	1.4775	-0.0001	0.4905	1.4772	0	0.4944
9B	0	0.8974	0.9899	0	0.8991	1.0249	0	0.9086	1.0473
10B	-1.4733	0	0.4682	-1.4775	0	0.4905	-1.4772	0	0.4944
11B	-0.9089	-1.4658	-0.4646	-0.9216	-1.4776	-0.4164	-0.933	-1.5111	-0.3843
12B	-0.0001	-0.8977	0.9899	0	-0.8992	1.0249	0	-0.9075	1.0479
13C	2.7709	0.0002	-2.1724	2.7367	0.0001	-2.2108	2.6946	-0.0008	-2.2687
14C	1.6993	2.798	-0.4611	1.7071	2.7969	-0.4619	1.7438	2.8016	-0.4338
15C	-1.699	2.7982	-0.4612	-1.7069	2.797	-0.4619	-1.7437	2.8016	-0.4337
16C	-2.7707	0.0005	-2.1726	-2.7367	0.0003	-2.2108	-2.6947	-0.0008	-2.2687
17C	1.6993	-2.7982	-0.4617	1.7071	-2.7973	-0.462	1.7431	-2.8023	-0.4319
18C	2.7651	-0.0002	1.3167	2.7787	0	1.3079	2.8033	0.0005	1.2514
19C	0	1.7154	2.3002	0.0001	1.715	2.328	0	1.6992	2.3539
20C	-2.7652	0.0001	1.3165	-2.7788	0.0003	1.3079	-2.8033	0.0006	1.2514
21C	-1.6995	-2.798	-0.4619	-1.7074	-2.7971	-0.462	-2.8023	-0.4318	
22C	-0.0002	-1.716	2.3	-0.0001	-1.7152	2.328	0	-1.6969	2.3553
24N	-3.7494	0.0001	1.937	-3.7719	0.0005	1.9121	-3.8164	0.001	1.823
25N	2.2965	3.7963	-0.4875	2.3016	3.7939	-0.5225	2.3578	3.7868	-0.492
26N	3.7313	0.0004	-2.8299	3.6573	0.0005	-2.9207	3.585	-0.0009	-3.0162
27N	-3.7309	0.0008	-2.8303	-3.6572	0.0008	-2.9209	-3.5851	-0.0009	-3.0161
28N	-2.2958	3.7966	-0.4874	-2.3011	3.7942	-0.5222	-2.3577	3.7868	-0.492
29N	-0.0003	2.3347	3.2848	0	2.3371	3.3098	0.0001	2.3078	3.345
30N	-2.2967	-3.7963	-0.4882	-2.3017	-3.7943	-0.5225	-2.3566	-3.7878	-0.49
31N	-0.0004	-2.3356	3.2844	-0.0001	-2.3374	3.3097	0	-2.3045	3.3471
32N	3.7492	-0.0002	1.9375	3.7718	0.0003	1.9124	3.8164	0.0009	1.8231
33N	2.2964	-3.7965	-0.488	2.3015	-3.7944	-0.5225	2.3565	-3.7879	-0.49

SII.2 Hirshfeld charges and condensed Fukui functions

Table S10: Hirshfeld charges and condensed Fukui functions for nucleophilic attack for species of the $[B_{12}Br_{11}]^q$ type ($q = 2\text{-}, 1\text{-}, 0$). All quantities are given in units of e (elementary charge). Given a particular charge q, the Hirshfeld charges for the systems with N and $N+1$ are computed at the optimized geometry for the system with N electrons shown in Table S2.

Atom/Total	$[B_{12}Br_{11}]^{2-}$ q_N	q_{N+1}	f^+	$[B_{12}Br_{11}]^{-}$ q_N	q_{N+1}	f^+	$B_{12}Br_{11}$ q_N	q_{N+1}	f^+
1B	-0.0580	-0.2026	0.1446	0.1470	-0.0858	0.2328	0.1551	0.1427	0.0124
2B	-0.0188	-0.0271	0.0084	-0.0123	-0.0159	0.0037	0.0044	-0.0139	0.0183
3B	-0.0187	-0.0271	0.0084	-0.0123	-0.0160	0.0037	-0.0040	-0.0142	0.0101
4B	-0.0188	-0.0272	0.0084	-0.0123	-0.0160	0.0037	-0.0065	-0.0145	0.0081
5B	-0.0188	-0.0272	0.0084	-0.0124	-0.0161	0.0037	-0.0060	-0.0146	0.0085
6B	-0.0187	-0.0271	0.0084	-0.0123	-0.0160	0.0037	-0.0048	-0.0141	0.0093
7B	-0.0167	-0.0228	0.0061	-0.0144	-0.0206	0.0062	-0.0090	-0.0163	0.0073
8B	-0.0166	-0.0228	0.0061	-0.0143	-0.0205	0.0062	-0.0072	-0.0167	0.0095
9B	-0.0167	-0.0228	0.0061	-0.0144	-0.0206	0.0062	-0.0020	-0.0159	0.0138
10B	-0.0166	-0.0228	0.0061	-0.0143	-0.0205	0.0062	-0.0063	-0.0166	0.0103
11B	-0.0167	-0.0228	0.0061	-0.0143	-0.0205	0.0062	-0.0096	-0.0165	0.0068
12B	-0.0187	-0.0214	0.0027	-0.0190	-0.0231	0.0040	-0.0200	-0.0214	0.0014
13Br	-0.1663	-0.2500	0.0838	-0.0880	-0.1575	0.0695	-0.0112	-0.0866	0.0753
14Br	-0.1663	-0.2501	0.0837	-0.0880	-0.1575	0.0695	-0.0154	-0.0860	0.0705
15Br	-0.1663	-0.2501	0.0837	-0.0880	-0.1576	0.0695	-0.0137	-0.0858	0.0721
16Br	-0.1663	-0.2500	0.0838	-0.0880	-0.1575	0.0695	-0.0134	-0.0868	0.0734
17Br	-0.1529	-0.2165	0.0636	-0.0913	-0.1545	0.0632	-0.0066	-0.0890	0.0824
18Br	-0.1529	-0.2165	0.0636	-0.0912	-0.1544	0.0632	-0.0022	-0.0887	0.0865
19Br	-0.1530	-0.2165	0.0636	-0.0914	-0.1545	0.0632	0.0122	-0.0877	0.0999
20Br	-0.1529	-0.2165	0.0636	-0.0913	-0.1545	0.0632	-0.0002	-0.0885	0.0883
21Br	-0.1529	-0.2165	0.0636	-0.0913	-0.1545	0.0632	-0.0079	-0.0892	0.0812
22Br	-0.1497	-0.1918	0.0421	-0.0982	-0.1483	0.0501	-0.0321	-0.0967	0.0646
23Br	-0.1663	-0.2501	0.0837	-0.0881	-0.1576	0.0696	0.0064	-0.0834	0.0898
Core total	-0.25	-0.47	0.22	-0.01	-0.29	0.29	0.08	-0.03	0.12
Subs. total	-1.75	-2.52	0.78	-0.99	-1.71	0.71	-0.08	-0.97	0.88
Total	-2.00	-3.00	1.00	-1.00	-2.00	1.00	0.00	-1.00	1.00

Table S11: Hirshfeld charges and condensed Fukui functions for nucleophilic attack for species of the $[B_{12}I_{11}]^q$ type (q = 2-, 1-, 0). All quantities are given in units of e (elementary charge). Given a particular charge q, the Hirshfeld charges for the systems with N and $N+1$ are computed at the optimized geometry for the system with N electrons shown in Table S3.

	$[B_{12}I_{11}]^{2-}$			$[B_{12}I_{11}]^{-}$			$B_{12}I_{11}$		
Atom/Total	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+
1B	-0.0557	-0.1504	0.0947	0.1208	-0.0769	0.1977	0.1307	0.1230	0.0077
2B	-0.0425	-0.0462	0.0037	-0.0436	-0.0417	-0.0019	-0.0478	-0.0448	-0.0030
3B	-0.0425	-0.0462	0.0037	-0.0437	-0.0418	-0.0019	-0.0478	-0.0448	-0.0030
4B	-0.0424	-0.0462	0.0037	-0.0437	-0.0418	-0.0019	-0.0478	-0.0448	-0.0030
5B	-0.0425	-0.0462	0.0037	-0.0437	-0.0418	-0.0019	-0.0478	-0.0448	-0.0030
6B	-0.0424	-0.0461	0.0037	-0.0437	-0.0418	-0.0019	-0.0477	-0.0448	-0.0030
7B	-0.0409	-0.0435	0.0026	-0.0426	-0.0446	0.0020	-0.0476	-0.0453	-0.0022
8B	-0.0409	-0.0435	0.0026	-0.0425	-0.0445	0.0020	-0.0475	-0.0453	-0.0022
9B	-0.0409	-0.0435	0.0026	-0.0426	-0.0446	0.0020	-0.0476	-0.0454	-0.0022
10B	-0.0410	-0.0435	0.0026	-0.0425	-0.0445	0.0020	-0.0476	-0.0453	-0.0022
11B	-0.0409	-0.0435	0.0026	-0.0426	-0.0446	0.0020	-0.0477	-0.0454	-0.0022
12B	-0.0439	-0.0431	-0.0007	-0.0474	-0.0477	0.0004	-0.0523	-0.0464	-0.0060
13I	-0.1440	-0.2385	0.0945	-0.0534	-0.1341	0.0807	0.0323	-0.0513	0.0836
14I	-0.1440	-0.2385	0.0945	-0.0534	-0.1341	0.0807	0.0323	-0.0513	0.0836
15I	-0.1440	-0.2385	0.0945	-0.0533	-0.1340	0.0807	0.0323	-0.0512	0.0836
16I	-0.1440	-0.2385	0.0945	-0.0534	-0.1341	0.0807	0.0324	-0.0513	0.0836
17I	-0.1440	-0.2385	0.0945	-0.0534	-0.1340	0.0806	0.0324	-0.0513	0.0837
18I	-0.1279	-0.1991	0.0712	-0.0617	-0.1304	0.0687	0.0523	-0.0617	0.1140
19I	-0.1279	-0.1992	0.0713	-0.0616	-0.1303	0.0687	0.0523	-0.0617	0.1140
20I	-0.1279	-0.1992	0.0713	-0.0617	-0.1303	0.0687	0.0523	-0.0617	0.1140
21I	-0.1279	-0.1992	0.0713	-0.0617	-0.1303	0.0687	0.0523	-0.0617	0.1139
22I	-0.1279	-0.1992	0.0712	-0.0616	-0.1303	0.0686	0.0523	-0.0617	0.1140
23I	-0.1232	-0.1673	0.0441	-0.0667	-0.1210	0.0543	-0.0254	-0.0614	0.0361
Core total	-0.52	-0.64	0.13	-0.36	-0.56	0.20	-0.40	-0.37	-0.02
Subs. total	-1.48	-2.36	0.87	-0.64	-1.44	0.80	0.40	-0.63	1.02
Total	-2.00	-3.00	1.00	-1.00	-2.00	1.00	0.00	-1.00	1.00

Table S12: Hirshfeld charges and condensed Fukui functions for nucleophilic attack for species of the $[B_{12}(CN)_{11}]^q$ type (q = 2-, 1-, 0). All quantities are given in units of e (elementary charge). Given a particular charge q, the Hirshfeld charges for the systems with N and $N+1$ are computed at the optimized geometry for the system with N electrons shown in Table S4.

Atom/Total	$[B_{12}(CN)_{11}]^{2-}$			$[B_{12}(CN)_{11}]^{-}$			$B_{12}(CN)_{11}$		
	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+
1B	-0.0204	-0.3056	0.2851	0.2070	-0.0706	0.2777	0.2201	0.2047	0.0154
2B	0.0228	0.0096	0.0131	0.0446	0.0341	0.0105	0.0582	0.0451	0.0131
3B	0.0228	0.0096	0.0131	0.0445	0.0340	0.0105	0.0604	0.0457	0.0147
4B	0.0228	0.0097	0.0131	0.0446	0.0341	0.0105	0.0688	0.0458	0.0230
5B	0.0228	0.0097	0.0131	0.0447	0.0342	0.0105	0.0604	0.0457	0.0147
6B	0.0228	0.0097	0.0131	0.0446	0.0342	0.0105	0.0582	0.0451	0.0131
7B	0.0293	0.0163	0.0130	0.0422	0.0284	0.0138	0.0568	0.0425	0.0143
8B	0.0294	0.0164	0.0131	0.0423	0.0285	0.0138	0.0543	0.0430	0.0113
9B	0.0293	0.0163	0.0131	0.0423	0.0285	0.0138	0.0543	0.0430	0.0114
10B	0.0293	0.0163	0.0130	0.0422	0.0284	0.0138	0.0568	0.0425	0.0143
11B	0.0294	0.0163	0.0131	0.0422	0.0284	0.0138	0.0611	0.0431	0.0180
12B	0.0275	0.0186	0.0088	0.0339	0.0246	0.0094	0.0401	0.0342	0.0059
13C	0.0196	0.0178	0.0018	0.0190	0.0209	-0.0019	0.0247	0.0178	0.0069
14C	0.0196	0.0178	0.0018	0.0189	0.0208	-0.0019	0.0269	0.0173	0.0096
15C	0.0196	0.0178	0.0018	0.0190	0.0209	-0.0019	0.0339	0.0168	0.0171
16C	0.0196	0.0178	0.0018	0.0190	0.0208	-0.0019	0.0269	0.0173	0.0096
17C	0.0196	0.0178	0.0018	0.0190	0.0208	-0.0019	0.0247	0.0178	0.0069
18C	0.0196	0.0174	0.0022	0.0196	0.0176	0.0020	0.0359	0.0181	0.0177
19C	0.0197	0.0175	0.0022	0.0196	0.0176	0.0020	0.0318	0.0183	0.0135
20C	0.0196	0.0175	0.0022	0.0196	0.0176	0.0020	0.0318	0.0183	0.0135
21C	0.0197	0.0175	0.0022	0.0196	0.0176	0.0020	0.0359	0.0182	0.0177
22C	0.0197	0.0175	0.0022	0.0197	0.0176	0.0020	0.0416	0.0176	0.0239
23C	0.0203	0.0207	-0.0004	0.0198	0.0191	0.0007	0.0235	0.0193	0.0042
24N	-0.2225	-0.2707	0.0482	-0.1731	-0.2249	0.0519	-0.1038	-0.1718	0.0680
25N	-0.2294	-0.2833	0.0539	-0.1686	-0.2252	0.0565	-0.1121	-0.1679	0.0558
26N	-0.2294	-0.2833	0.0539	-0.1687	-0.2252	0.0566	-0.0966	-0.1670	0.0705
27N	-0.2294	-0.2833	0.0539	-0.1686	-0.2252	0.0565	-0.1084	-0.1681	0.0597
28N	-0.2294	-0.2833	0.0539	-0.1686	-0.2251	0.0565	-0.1121	-0.1679	0.0558
29N	-0.2294	-0.2833	0.0539	-0.1686	-0.2252	0.0565	-0.1083	-0.1681	0.0597
30N	-0.2225	-0.2707	0.0482	-0.1731	-0.2249	0.0519	-0.1093	-0.1719	0.0625
31N	-0.2225	-0.2707	0.0482	-0.1730	-0.2249	0.0519	-0.0951	-0.1714	0.0763
32N	-0.2219	-0.2657	0.0437	-0.1773	-0.2246	0.0473	-0.1259	-0.1765	0.0506
33N	-0.2225	-0.2707	0.0482	-0.1731	-0.2249	0.0519	-0.1093	-0.1719	0.0625
34N	-0.2225	-0.2707	0.0482	-0.1731	-0.2250	0.0519	-0.1038	-0.1718	0.0680
Core total	0.27	-0.16	0.42	0.68	0.27	0.41	0.85	0.68	0.17
Subs. total	-2.26	-2.84	0.57	-1.67	-2.26	0.59	-0.85	-1.68	0.83
Total	-2.00	-3.00	1.00	-1.00	-2.00	1.00	0.00	-1.00	1.00

Table S13: Hirshfeld charges and condensed Fukui functions for nucleophilic attack for species of the $[B_{12}Br_{10}]^q$ type (q = 2-, 1-, 0). All quantities are given in units of e (elementary charge). Given a particular charge q, the Hirshfeld charges for the systems with N and $N+1$ are computed at the optimized geometry for the system with N electrons shown in Table S5.

Atom/Total	$[B_{12}Br_{10}]^{2-}$ q_N	q_{N+1}	f^+	$[B_{12}Br_{10}]^-$ q_N	q_{N+1}	f^+	$B_{12}Br_{10}$ q_N	q_{N+1}	f^+
1B	-0.0594	-0.1930	0.1336	0.0583	-0.0689	0.1271	0.1472	0.0460	0.1012
2B	-0.0594	-0.1930	0.1336	0.0583	-0.0689	0.1271	0.1472	0.0460	0.1012
3B	-0.0186	-0.0239	0.0052	-0.0126	-0.0191	0.0065	-0.0070	-0.0111	0.0041
4B	-0.0072	-0.0186	0.0114	-0.0072	-0.0116	0.0044	-0.0048	-0.0076	0.0028
5B	-0.0072	-0.0186	0.0114	-0.0072	-0.0116	0.0044	-0.0048	-0.0076	0.0028
6B	-0.0186	-0.0239	0.0052	-0.0126	-0.0191	0.0065	-0.0070	-0.0111	0.0041
7B	-0.0072	-0.0186	0.0114	-0.0072	-0.0116	0.0044	-0.0048	-0.0076	0.0028
8B	-0.0118	-0.0169	0.0052	-0.0114	-0.0181	0.0067	-0.0086	-0.0159	0.0072
9B	-0.0165	-0.0250	0.0085	-0.0151	-0.0194	0.0043	-0.0101	-0.0162	0.0061
10B	-0.0118	-0.0169	0.0052	-0.0114	-0.0181	0.0067	-0.0086	-0.0158	0.0072
11B	-0.0072	-0.0186	0.0114	-0.0072	-0.0116	0.0044	-0.0048	-0.0076	0.0028
12B	-0.0165	-0.0250	0.0085	-0.0151	-0.0194	0.0043	-0.0101	-0.0162	0.0061
13Br	-0.2106	-0.2766	0.0660	-0.1085	-0.1957	0.0872	-0.0148	-0.1027	0.0879
14Br	-0.1780	-0.2472	0.0691	-0.1016	-0.1716	0.0700	-0.0285	-0.0959	0.0675
15Br	-0.1780	-0.2472	0.0691	-0.1016	-0.1716	0.0700	-0.0285	-0.0959	0.0675
16Br	-0.2106	-0.2766	0.0660	-0.1084	-0.1957	0.0872	-0.0148	-0.1027	0.0879
17Br	-0.1780	-0.2472	0.0691	-0.1016	-0.1716	0.0700	-0.0285	-0.0959	0.0675
18Br	-0.1609	-0.2142	0.0532	-0.0970	-0.1621	0.0651	-0.0175	-0.1005	0.0830
19Br	-0.1515	-0.2182	0.0667	-0.0961	-0.1502	0.0541	-0.0226	-0.0925	0.0699
20Br	-0.1609	-0.2142	0.0532	-0.0970	-0.1621	0.0651	-0.0175	-0.1005	0.0830
21Br	-0.1780	-0.2472	0.0691	-0.1016	-0.1716	0.0700	-0.0285	-0.0959	0.0675
22Br	-0.1515	-0.2182	0.0667	-0.0961	-0.1502	0.0541	-0.0226	-0.0925	0.0699
Core total	-0.24	-0.59	0.35	0.01	-0.30	0.31	0.22	-0.02	0.25
Subs. total	-1.76	-2.41	0.65	-1.01	-1.70	0.69	-0.22	-0.98	0.75
Total	-2.00	-3.00	1.00	-1.00	-2.00	1.00	0.00	-1.00	1.00

Table S14: Hirshfeld charges and condensed Fukui functions for nucleophilic attack for species of the $[B_{12}I_{10}]^q$ type ($q = 2-, 1-, 0$). All quantities are given in units of e (elementary charge). Given a particular charge q, the Hirshfeld charges for the systems with N and $N+1$ are computed at the optimized geometry for the system with N electrons shown in Table S6.

Atom/Total	$[B_{12}I_{10}]^{2-}$			$[B_{12}I_{10}]^{-}$			$B_{12}I_{10}$		
	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+
1B	-0.0513	-0.1622	0.1109	0.0410	-0.0603	0.1013	0.1064	0.0301	0.0763
2B	-0.0513	-0.1622	0.1109	0.0410	-0.0603	0.1013	0.1064	0.0301	0.0763
3B	-0.0368	-0.0369	0.0001	-0.0411	-0.0412	0.0000	-0.0433	-0.0418	-0.0015
4B	-0.0305	-0.0373	0.0068	-0.0367	-0.0361	-0.0006	-0.0408	-0.0386	-0.0022
5B	-0.0305	-0.0373	0.0068	-0.0367	-0.0361	-0.0006	-0.0408	-0.0386	-0.0022
6B	-0.0368	-0.0369	0.0001	-0.0411	-0.0412	0.0000	-0.0433	-0.0418	-0.0015
7B	-0.0305	-0.0373	0.0068	-0.0367	-0.0361	-0.0006	-0.0408	-0.0386	-0.0022
8B	-0.0348	-0.0361	0.0013	-0.0384	-0.0407	0.0023	-0.0391	-0.0413	0.0021
9B	-0.0410	-0.0466	0.0056	-0.0434	-0.0438	0.0004	-0.0434	-0.0440	0.0006
10B	-0.0348	-0.0361	0.0013	-0.0384	-0.0407	0.0023	-0.0391	-0.0413	0.0021
11B	-0.0305	-0.0373	0.0068	-0.0367	-0.0361	-0.0006	-0.0408	-0.0386	-0.0022
12B	-0.0410	-0.0466	0.0056	-0.0434	-0.0438	0.0004	-0.0434	-0.0440	0.0006
13I	-0.2010	-0.2760	0.0750	-0.0724	-0.1810	0.1086	0.0499	-0.0630	0.1129
14I	-0.1570	-0.2334	0.0765	-0.0701	-0.1497	0.0797	0.0141	-0.0654	0.0795
15I	-0.1570	-0.2334	0.0765	-0.0701	-0.1497	0.0797	0.0141	-0.0654	0.0795
16I	-0.2010	-0.2760	0.0750	-0.0724	-0.1810	0.1086	0.0499	-0.0630	0.1129
17I	-0.1570	-0.2334	0.0765	-0.0701	-0.1497	0.0797	0.0141	-0.0654	0.0795
18I	-0.1372	-0.1967	0.0595	-0.0673	-0.1389	0.0715	0.0160	-0.0705	0.0865
19I	-0.1222	-0.2023	0.0802	-0.0643	-0.1219	0.0576	0.0074	-0.0610	0.0684
20I	-0.1372	-0.1967	0.0595	-0.0673	-0.1389	0.0715	0.0160	-0.0705	0.0865
21I	-0.1570	-0.2334	0.0765	-0.0701	-0.1497	0.0797	0.0141	-0.0654	0.0795
22I	-0.1222	-0.2023	0.0802	-0.0643	-0.1219	0.0576	0.0074	-0.0610	0.0684
Core total	-0.45	-0.71	0.26	-0.31	-0.52	0.21	-0.20	-0.35	0.15
Subs. total	-1.55	-2.28	0.74	-0.69	-1.48	0.79	0.20	-0.65	0.85
Total	-2.00	-3.00	1.00	-1.00	-2.00	1.00	0.00	-1.00	1.00

Table S15: Hirshfeld charges and condensed Fukui functions for nucleophilic attack for species of the $[B_{12}(CN)_{10}]^q$ type (q = 2-, 1-, 0). All quantities are given in units of e (elementary charge). Given a particular charge q, the Hirshfeld charges for the systems with N and $N+1$ are computed at the optimized geometry for the system with N electrons shown in Table S7.

Atom/Total	$[B_{12}(CN)_{10}]^{2-}$			$[B_{12}(CN)_{10}]^{-}$			$B_{12}(CN)_{10}$		
	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+	q_N	q_{N+1}	f^+
1B	-0.0476	-0.2194	0.1718	0.1063	-0.0542	0.1605	0.2206	0.0922	0.1284
2B	-0.0476	-0.2194	0.1718	0.1062	-0.0542	0.1605	0.2207	0.0922	0.1285
3B	0.0150	0.0032	0.0117	0.0370	0.0233	0.0136	0.0552	0.0438	0.0114
4B	0.0340	0.0164	0.0176	0.0459	0.0347	0.0112	0.0605	0.0503	0.0102
5B	0.0340	0.0164	0.0176	0.0459	0.0347	0.0112	0.0605	0.0503	0.0102
6B	0.0150	0.0032	0.0117	0.0370	0.0233	0.0136	0.0552	0.0438	0.0114
7B	0.0340	0.0164	0.0176	0.0459	0.0348	0.0112	0.0605	0.0503	0.0102
8B	0.0316	0.0178	0.0138	0.0432	0.0283	0.0149	0.0557	0.0393	0.0164
9B	0.0248	0.0118	0.0130	0.0364	0.0253	0.0110	0.0508	0.0375	0.0133
10B	0.0316	0.0178	0.0138	0.0432	0.0283	0.0149	0.0557	0.0393	0.0164
11B	0.0340	0.0164	0.0176	0.0459	0.0348	0.0112	0.0605	0.0503	0.0102
12B	0.0249	0.0119	0.0130	0.0364	0.0253	0.0110	0.0507	0.0373	0.0133
13C	0.0151	0.0180	-0.0029	0.0165	0.0150	0.0015	0.0186	0.0154	0.0032
14C	0.0167	0.0171	-0.0004	0.0175	0.0168	0.0007	0.0198	0.0182	0.0016
15C	0.0167	0.0171	-0.0004	0.0175	0.0168	0.0007	0.0198	0.0182	0.0016
16C	0.0151	0.0180	-0.0029	0.0165	0.0150	0.0015	0.0186	0.0154	0.0032
17C	0.0167	0.0171	-0.0004	0.0175	0.0168	0.0007	0.0198	0.0182	0.0016
18C	0.0178	0.0151	0.0026	0.0183	0.0160	0.0023	0.0228	0.0148	0.0080
19C	0.0195	0.0170	0.0025	0.0193	0.0188	0.0005	0.0232	0.0181	0.0051
20C	0.0178	0.0151	0.0026	0.0183	0.0160	0.0023	0.0228	0.0148	0.0080
21C	0.0167	0.0171	-0.0004	0.0175	0.0168	0.0007	0.0198	0.0182	0.0016
22C	0.0195	0.0170	0.0025	0.0193	0.0188	0.0005	0.0232	0.0181	0.0051
24N	-0.2288	-0.2793	0.0505	-0.1791	-0.2311	0.0520	-0.1211	-0.1815	0.0604
25N	-0.2354	-0.2858	0.0504	-0.1797	-0.2345	0.0548	-0.1215	-0.1768	0.0553
26N	-0.2476	-0.2997	0.0522	-0.1835	-0.2444	0.0609	-0.1192	-0.1813	0.0621
27N	-0.2476	-0.2997	0.0522	-0.1835	-0.2444	0.0609	-0.1192	-0.1813	0.0621
28N	-0.2354	-0.2858	0.0504	-0.1797	-0.2345	0.0548	-0.1215	-0.1768	0.0553
29N	-0.2285	-0.2774	0.0489	-0.1805	-0.2295	0.0491	-0.1231	-0.1802	0.0571
30N	-0.2354	-0.2858	0.0504	-0.1797	-0.2345	0.0548	-0.1216	-0.1768	0.0553
31N	-0.2285	-0.2773	0.0489	-0.1805	-0.2296	0.0491	-0.1232	-0.1803	0.0571
32N	-0.2288	-0.2793	0.0505	-0.1791	-0.2311	0.0520	-0.1211	-0.1815	0.0604
33N	-0.2354	-0.2858	0.0504	-0.1797	-0.2345	0.0548	-0.1216	-0.1768	0.0553
Core total	0.18	-0.31	0.49	0.63	0.18	0.44	1.01	0.63	0.38
Subs. total	-2.18	-2.69	0.51	-1.63	-2.18	0.55	-1.00	-1.62	0.62
Total	-2.00	-2.99	1.00	-1.00	-2.00	1.00	0.00	-1.00	1.00

SIII Geometries and frequencies of the TSs associated with Coulomb barriers

SIII.1 TS for the B–Br cleavage in $[B_{12}Br_{12}]^{2-}$

Table S16: Relaxed scan of the B1-Br23 distance in $[B_{12}Br_{12}]^{2-}$. The energy is relative to the energy of the optimized species with a B1-Br23 equilibrium bond length of 1.97 Å. The line in bold face corresponds to the geometry taken as a guess for the transition state optimization. The natural charge for Br23 was -0.60 e at a B1-Br23 distance of 3.37 Å. The numbering of the atoms corresponds to the geometries given in Section SI.1.

B1-Br23 dist. (Å)	Energy (eV)
1.07	33.4916
1.17	21.1632
1.27	13.0344
1.37	7.7581
1.47	4.3971
1.57	2.3142
1.67	1.0800
1.77	0.4020
1.87	0.0848
1.97	0.0000
2.07	0.0644
2.17	0.2244
2.27	0.4419
2.37	0.6902
2.47	0.9501
2.57	1.2086
2.67	1.4587
2.77	1.6962
2.87	1.9196
2.97	2.1277
3.07	2.3200
3.17	2.4962
3.27	2.6568
3.37	**2.8021**
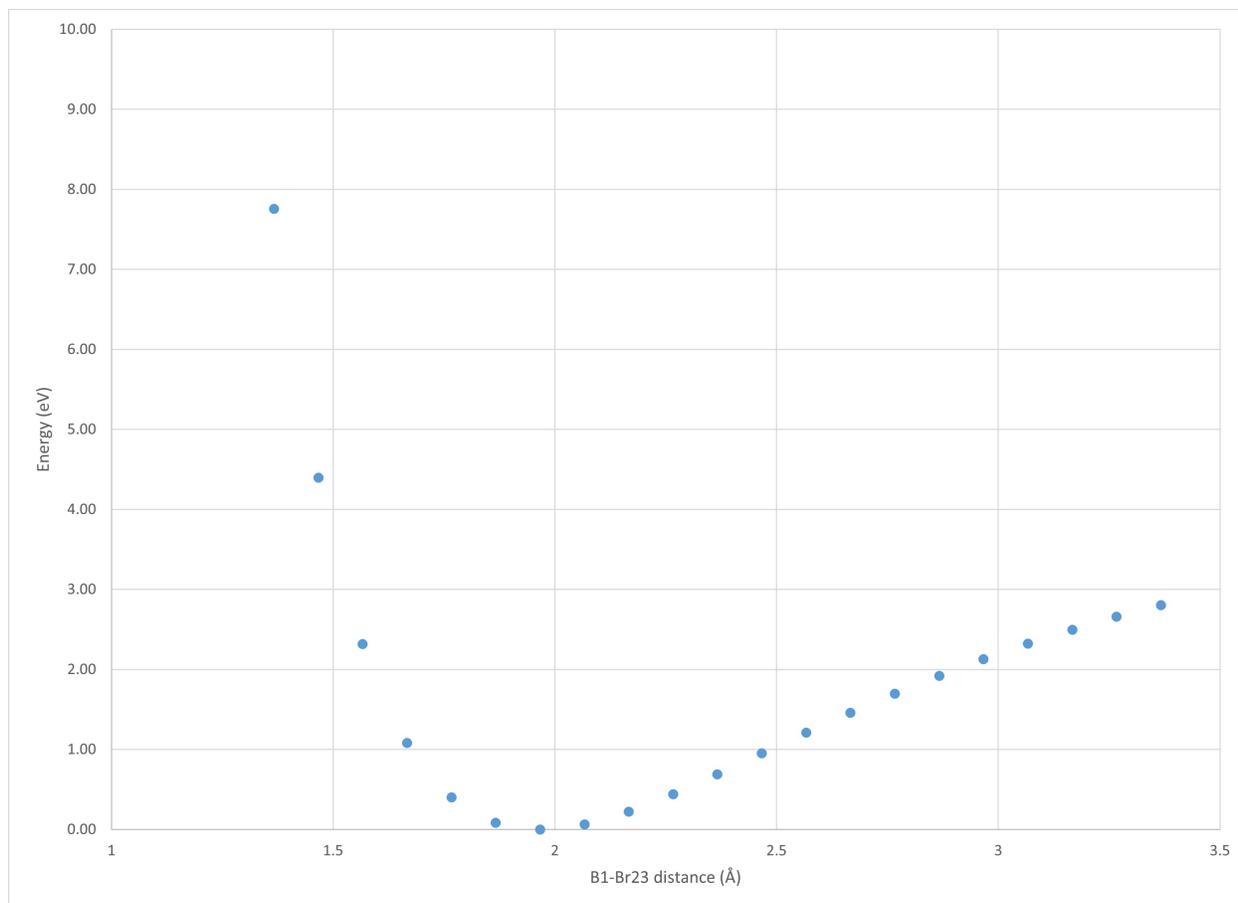
Figure S1: Plot of the relaxed scan of the B1-Br23 distance in $[B_{12}Br_{12}]^{2-}$ using the data in Table S14.

Table S17: Optimized geometry in Å for the transition state associated with the Coulomb barrier to break the B1-Br23 bond in $[B_{12}Br_{12}]^{2-}$.

Atom	x	y	z
B	1.2809	-0.0078	-0.0074
B	0.5259	-1.2920	-0.8692
B	0.5388	-1.2280	0.9530
B	0.5470	0.5249	1.4553
B	0.5392	1.5443	-0.0567
B	0.5260	0.4213	-1.4934
B	-0.9881	-1.5352	0.0625
B	-0.9753	-0.4245	1.4835
B	-0.9750	1.2703	0.8661
B	-0.9879	1.2069	-0.9364
B	-0.9960	-0.5270	-1.4330
B	-1.9150	0.0005	0.0151
Br	1.5077	-2.5675	1.9915
Br	1.5251	1.1028	3.0427
Br	1.5089	3.2369	-0.1226
Br	1.4813	0.8855	-3.1309
Br	-1.8685	-3.2823	0.1303
Br	-1.8408	-0.9044	3.1724
Br	-1.8408	2.7237	1.8508
Br	-1.8685	2.5881	-2.0081
Br	-1.8855	-1.1242	-3.0712
Br	-3.8743	0.0055	0.0290
Br	7.2995	0.0851	-0.0986
Br	1.4806	-2.7017	-1.8242

Table S18: Harmonic frequencies (cm^{-1}) and intensities $(\mathrm{km\ mol}^{-1})$ for the transition state associated with the Coulomb barrier to break the B1-Br23 bond in $[\mathrm{B}_{12}\mathrm{Br}_{12}]^{2-}$.

Frequency	Intensity	Frequency	Intensity
-19.9152	9.1268	384.0897	137.5870
3.5598	2.7624	431.3624	37.0082
3.9325	2.7611	431.4119	36.9626
63.8207	0.0000	538.4887	0.0010
63.9506	0.0000	538.9125	0.0052
72.0802	0.0000	544.1799	0.4943
75.5703	0.0017	544.2919	0.5095
75.5847	0.0019	546.0336	0.0088
81.9463	0.0000	594.7503	70.2267
82.0771	0.0000	635.0591	0.0003
83.9425	0.1798	635.181	0.0001
86.2326	0.0090	666.8945	1.6030
86.2676	0.0090	667.2568	1.6022
91.9785	0.0000	692.0017	0.0005
92.0433	0.0000	692.0414	0.0022
97.6616	0.0000	710.4901	1.6124
97.6839	0.0000	710.5886	1.6022
99.7181	0.0045	715.8053	0.0008
99.7499	0.0046	716.0985	0.0036
105.999	0.0708	790.4272	31.0957
106.0419	0.0707	790.6416	33.5372
107.5931	0.2680	792.1159	129.1928
185.3476	0.0473	884.2887	0.0060
185.4027	0.0475	884.6208	0.0020
191.1884	0.3174	898.9712	4.1903
191.2143	0.1241	930.9043	0.0383
191.2263	0.1788	931.0771	0.0139
200.6908	0.1215	941.9072	118.8905
206.5599	0.0000	942.2253	120.0078
206.5925	0.0000	945.8649	56.5847
343.6503	2.2718	960.7327	205.5274
344.0022	2.3045	986.5564	103.4897
366.7396	0.0081	986.7414	102.3084

SIII.2   TS for the B–Br cleavage in $[B_{12}Br_{11}]^{2-\bullet}$

Table S19:   Relaxed scan of the B2-Br23 distance in $[B_{12}Br_{11}]^{2-\bullet}$. The energy is relative to the energy of the optimized species with a B2-Br23 equilibrium bond length of 1.98 Å. The line in bold face corresponds to the geometry taken as a guess for the transition state optimization. The natural charge for Br23 was -0.62 e at a B2-Br23 distance of 3.68 Å. The numbering of the atoms corresponds to the geometries given in Section SI.1.

B2-Br23 dist. (Å)	Energy (eV)
1.18	19.9123
1.28	12.2470
1.38	7.2792
1.48	4.1190
1.58	2.1652
1.68	1.0091
1.78	0.3760
1.88	0.0798
1.98	0.0000
2.08	0.0594
2.18	0.2076
2.28	0.4077
2.38	0.6331
2.48	0.8663
2.58	1.0951
2.68	1.3131
2.78	1.5168
2.88	1.7052
2.98	1.7374
3.08	1.8967
3.18	2.0375
3.28	2.1553
3.38	2.2459
3.48	2.3239
3.58	2.3942
3.68	2.4558
3.73	**2.4839**
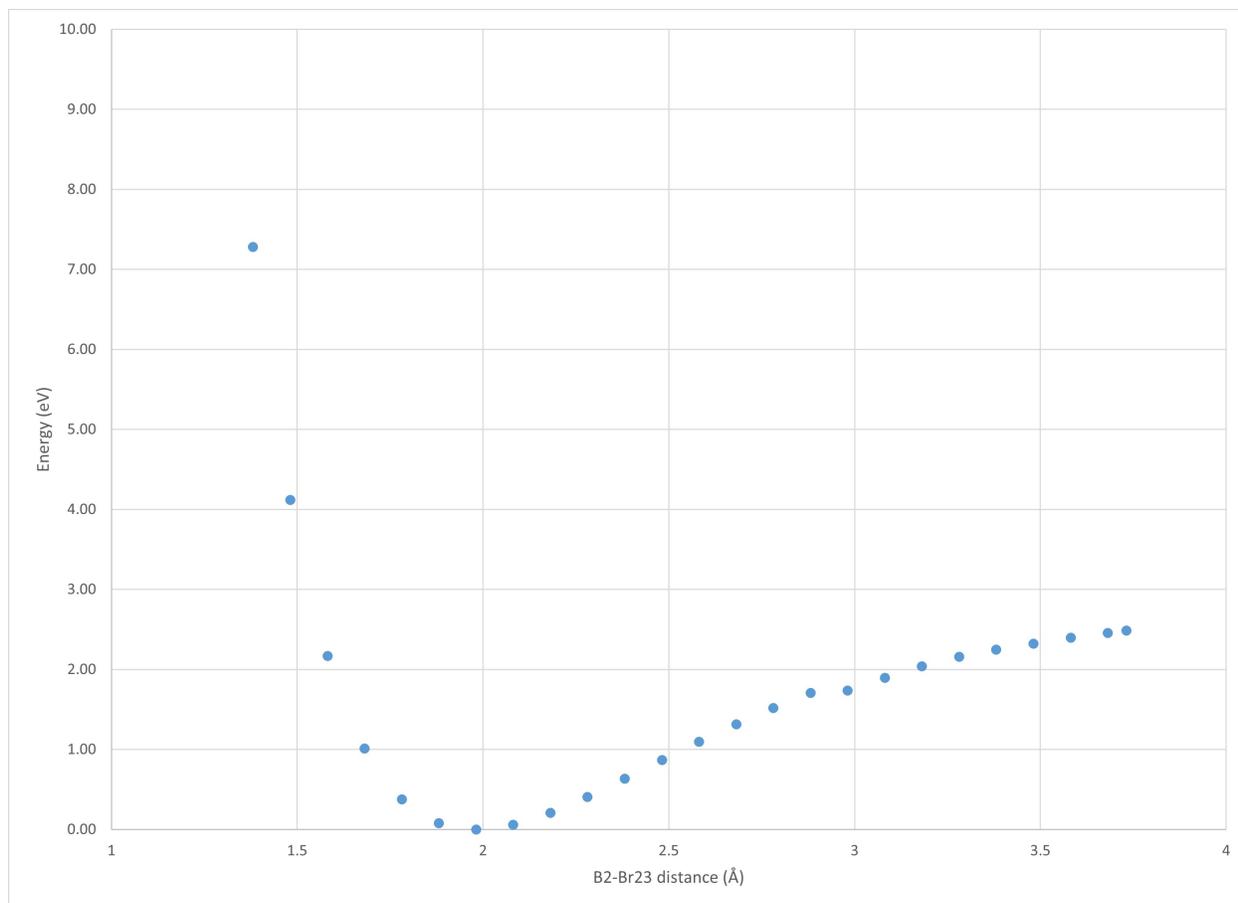
Figure S2: Plot of the relaxed scan of the B2-Br23 distance in $[\text{B}_{12}\text{Br}_{11}]^{2-\bullet}$ using the data in Table S17.

Table S20: Optimized geometry in Å for the transition state associated with the Coulomb barrier to break the B2-Br23 bond in $[B_{12}Br_{11}]^{2-\bullet}$.

Atom	x	y	z
B	-0.9609	0.0019	-1.2163
B	-1.4802	0.0022	0.2960
B	-0.8131	-1.4657	-0.3200
B	0.4978	-0.9123	-1.4174
B	0.5006	0.9117	-1.4168
B	-0.8086	1.4685	-0.3191
B	-0.4527	-0.9118	1.3510
B	0.8768	-1.4734	0.2602
B	1.6779	-0.0024	-0.4137
B	0.8813	1.4706	0.2611
B	-0.4499	0.9124	1.3515
B	1.0950	-0.0021	1.2835
Br	-1.8838	-3.0828	-0.6874
Br	1.0089	-1.9316	-3.0201
Br	1.0148	1.9304	-3.0189
Br	-1.8743	3.0890	-0.6854
Br	-1.0338	-1.9302	2.9302
Br	1.8573	-3.1381	0.5973
Br	3.5933	-0.0052	-0.8435
Br	1.8669	3.1320	0.5992
Br	-1.0278	1.9316	2.9314
Br	2.3428	-0.0045	2.7990
Br	-6.6941	0.0108	-2.3219

Table S21: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition state associated with the Coulomb barrier to break the B2-Br23 bond in $[\text{B}_{12}\text{Br}_{11}]^{2-\bullet}$.

Frequency	Intensity	Frequency	Intensity
-17.0955	5.7968	423.2874	48.1301
7.4629	1.4820	524.3197	103.3544
13.9277	1.3865	542.4503	0.0363
67.2169	0.0000	544.9054	2.0199
70.3672	0.0089	549.0650	0.0000
70.6827	0.2033	562.0653	0.0001
79.8792	0.0000	564.7024	22.5056
81.0165	0.0003	621.3347	0.0096
81.9256	0.0081	658.8768	0.1476
84.4366	0.0215	662.1236	0.0097
88.1696	0.0979	664.3403	4.3412
91.1395	0.0000	703.4573	0.0071
93.1050	0.0447	709.6569	0.5619
100.4375	0.0003	713.3785	0.9538
100.9754	0.0000	716.8302	0.0001
101.3186	0.0000	744.9646	13.3566
101.9023	0.0442	757.0634	51.9367
106.7478	0.1993	785.7448	0.0249
106.7650	0.2029	790.5304	12.6600
110.8639	0.6693	807.9981	0.0001
187.6129	4.8646	864.2965	15.4375
187.7680	0.0239	869.0051	0.0016
190.4966	1.0197	904.6280	68.4524
191.5710	0.0000	906.8914	0.3707
198.1078	0.0617	929.8041	69.4291
200.4737	0.0388	931.6355	409.0629
202.3568	0.0078	942.3637	0.0755
335.0207	2.6664	951.6130	328.2990
339.9832	3.1156	952.8922	239.7407
357.9899	64.2064	974.3226	291.1214
362.5877	0.0009	1085.4557	250.8033
384.2263	1.4937		

SIII.3   TS for the B–I cleavage in $[B_{12}I_{12}]^{2-}$

Table S22: Relaxed scan of the B1-I13 distance in $[B_{12}I_{12}]^{2-}$. The energy is relative to the energy of the optimized species with a B1-I13 equilibrium bond length of 2.21 Å. The line in bold face corresponds to the geometry taken as a guess for the transition state optimization. The natural charge for I13 was -0.76 e at a B1-I13 distance of 7.62 Å. The numbering of the atoms corresponds to the geometries given in Section SI.1.

B1-I13 dist. (Å)	Energy (eV)	B1-I13 dist. (Å)	Energy (eV)
1.22	29.9071	4.52	2.3890
1.32	19.7904	4.62	2.4095
1.42	12.8354	4.72	2.4259
1.52	8.1057	4.82	2.4387
1.62	4.9379	4.92	2.4483
1.72	2.8613	5.02	2.4551
1.82	1.5400	5.12	2.4595
1.92	0.7340	5.22	2.4618
2.02	0.2782	**5.32**	**2.4623**
2.12	0.0597	5.42	2.4613
2.22	0.0000	5.52	2.4589
2.32	0.0436	5.62	2.4553
2.42	0.1545	5.72	2.4507
2.52	0.3052	5.82	2.4452
2.62	0.4773	5.92	2.4390
2.72	0.6592	6.02	2.4322
2.82	0.8411	6.12	2.4248
2.92	1.0182	6.22	2.4169
3.02	1.1867	6.32	2.4086
3.12	1.3441	6.42	2.4000
3.22	1.4892	6.52	2.3912
3.32	1.6215	6.62	2.3822
3.42	1.7411	6.72	2.3730
3.52	1.8484	6.82	2.3637
3.62	1.9440	6.92	2.3543
3.72	2.0284	7.02	2.3447
3.82	2.0984	7.12	2.3351
3.92	2.1634	7.22	2.3255
4.02	2.2200	7.32	2.3159
4.12	2.2687	7.42	2.3062
4.22	2.3105	7.52	2.2966
4.32	2.3460	7.62	2.2870
4.42	2.3758		
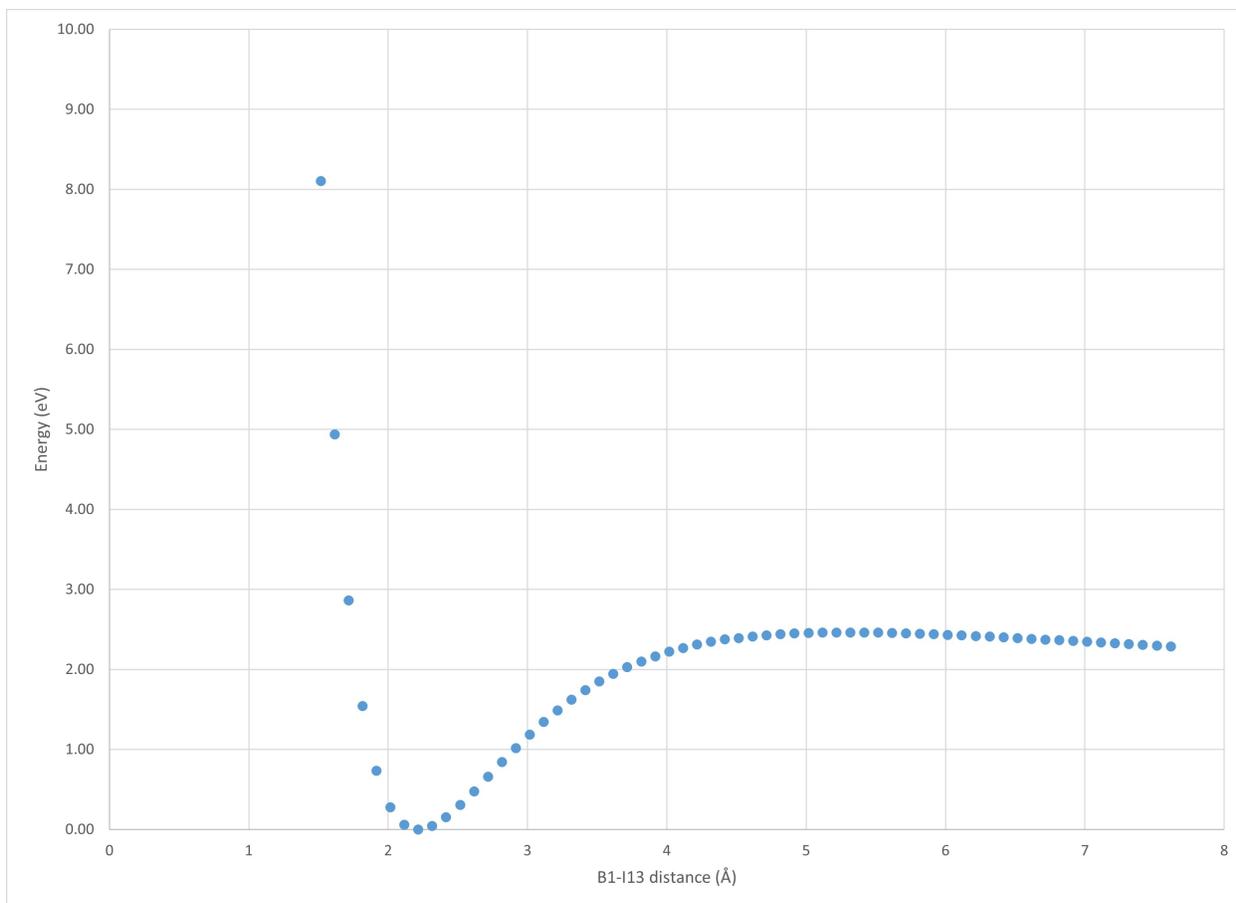
Figure S3: Plot of the relaxed scan of the B1-I13 distance in $[B_{12}I_{12}]^{2-}$ using the data in Table S20.

Table S23: Optimized geometry in Å for the transition state associated with the Coulomb barrier to break the B1-I13 bond in $[B_{12}I_{12}]^{2-}$.

Atom	x	y	z
B	-1.3079	0.0027	0.0001
B	-0.5645	-1.3377	0.7850
B	-0.5644	-1.1589	-1.0310
B	-0.5613	0.6234	-1.4222
B	-0.5597	1.5462	0.1522
B	-0.5616	0.3341	1.5162
B	0.9602	-1.5348	-0.1511
B	0.9622	-0.3315	-1.5055
B	0.9651	1.3284	-0.7794
B	0.9650	1.1509	1.0236
B	0.9620	-0.6187	1.4119
B	1.8969	-0.0027	-0.0002
I	-6.6056	0.0038	0.0006
I	-1.6653	-2.9791	1.7484
I	-1.6653	-2.5809	-2.2960
I	-1.6586	1.3885	-3.1672
I	-1.6553	3.4434	0.3387
I	-1.6592	0.7443	3.3767
I	1.9264	-3.5097	-0.3454
I	1.9309	-0.7581	-3.4422
I	1.9373	3.0375	-1.7821
I	1.9370	2.6315	2.3405
I	1.9303	-1.4148	3.2284
I	4.1065	-0.0064	-0.0004

Table S24: Harmonic frequencies (cm^{-1}) and intensities ($km\ mol^{-1}$) for the transition state associated with the Coulomb barrier to break the B1-I13 bond in $[B_{12}I_{12}]^{2-}$.

Frequency	Intensity	Frequency	Intensity
-19.9223	6.8221	353.6488	0.0116
9.5904	1.2327	361.0043	20.4201
9.6458	1.2324	361.0490	20.4119
45.1636	0.0000	529.8396	0.0131
45.2435	0.0000	530.3435	0.0102
51.2746	0.0000	531.8742	0.9414
54.5911	0.0050	532.0321	0.9977
54.6121	0.0050	532.5336	0.0587
58.5281	0.0000	561.8721	65.5793
58.5448	0.0000	607.9874	0.0003
63.3314	0.0082	608.0297	0.0001
63.3835	0.0139	624.3732	0.8552
63.4043	0.0132	624.4544	0.8463
69.2730	0.0000	684.3204	0.0016
69.2848	0.0000	684.6977	0.0111
70.7631	0.0061	687.9952	2.0955
70.7759	0.0061	688.1844	2.0549
74.7199	0.0000	709.0281	0.0028
74.7401	0.0000	709.3752	0.0006
81.4664	0.4523	742.8297	73.5271
81.4836	0.4531	772.8470	22.2167
82.0102	0.0012	773.1050	22.2798
135.0353	0.0028	816.2499	0.0026
135.0443	0.0027	816.9460	0.0007
137.2374	0.0002	848.6521	13.5575
137.2446	0.0000	869.3625	0.0332
137.6205	0.9043	869.3944	0.0424
141.6180	0.2846	873.8067	107.6305
144.6903	0.0000	881.9217	145.6770
144.7163	0.0000	882.3002	145.3877
322.3407	62.2638	895.3292	49.4031
325.0914	10.5000	944.8638	24.4516
325.1837	10.5281	944.9399	24.4955

SIII.4   TS for the B–I cleavage in $[B_{12}I_{11}]^{2-\bullet}$

Table S25: Relaxed scan of the B2-I13 distance in $[B_{12}I_{11}]^{2-\bullet}$. The energy is relative to the energy of the optimized species (with a B2-I13 equilibrium bond length of 2.23 Å. The line in bold face corresponds to the geometry taken as a guess for the transition state optimization. The natural charge for I13 was -0.64 e at a B2-I13 distance of 9.23 Å. The numbering of the atoms corresponds to the geometries given in Section SI.1.

B2-I13 dist. (Å)	Energy (eV)	B2-I13 dist. (Å)	Energy (eV)
1.33	18.7126	5.33	1.8630
1.43	12.1224	5.43	1.8568
1.53	7.6427	5.53	1.8499
1.63	4.6467	5.63	1.8425
1.73	2.6868	5.73	1.8346
1.83	1.4419	5.83	1.8263
1.93	0.6849	5.93	1.8176
2.03	0.2587	6.03	1.8087
2.13	0.0554	6.13	1.7996
2.23	0.0000	6.23	1.7904
2.33	0.0410	6.33	172.2848
2.43	0.1421	6.43	175.0060
2.53	0.2785	6.53	177.7271
2.63	0.4330	6.63	180.4483
2.73	0.5938	6.73	183.1694
2.83	0.7528	6.83	185.8906
2.93	0.9047	6.93	188.6118
3.03	1.0462	7.03	191.3329
3.13	1.1754	7.13	194.0541
3.23	1.2916	7.23	196.7752
3.33	1.3942	7.33	199.4964
3.43	1.4835	7.43	202.2176
3.53	1.5600	7.53	204.9387
3.63	1.6247	7.63	207.6599
3.73	1.6790	7.73	210.3810
3.83	1.7245	7.83	213.1022
3.93	1.7622	7.93	215.8234
4.03	1.7928	8.03	218.5445
4.13	1.8171	8.13	221.2657
4.23	1.8362	8.23	223.9868
4.33	1.8511	8.33	226.7080
4.43	1.8613	8.43	229.4292
4.53	1.8698	8.53	232.1503
4.63	1.8754	8.63	234.8715
4.73	1.8786	8.73	237.5926
4.83	**1.8795**	8.83	240.3138
4.93	1.8787	8.93	243.0350
5.03	1.8765	9.03	245.7561
5.13	1.8730	9.13	248.4773
5.23	1.8684	9.23	251.1984
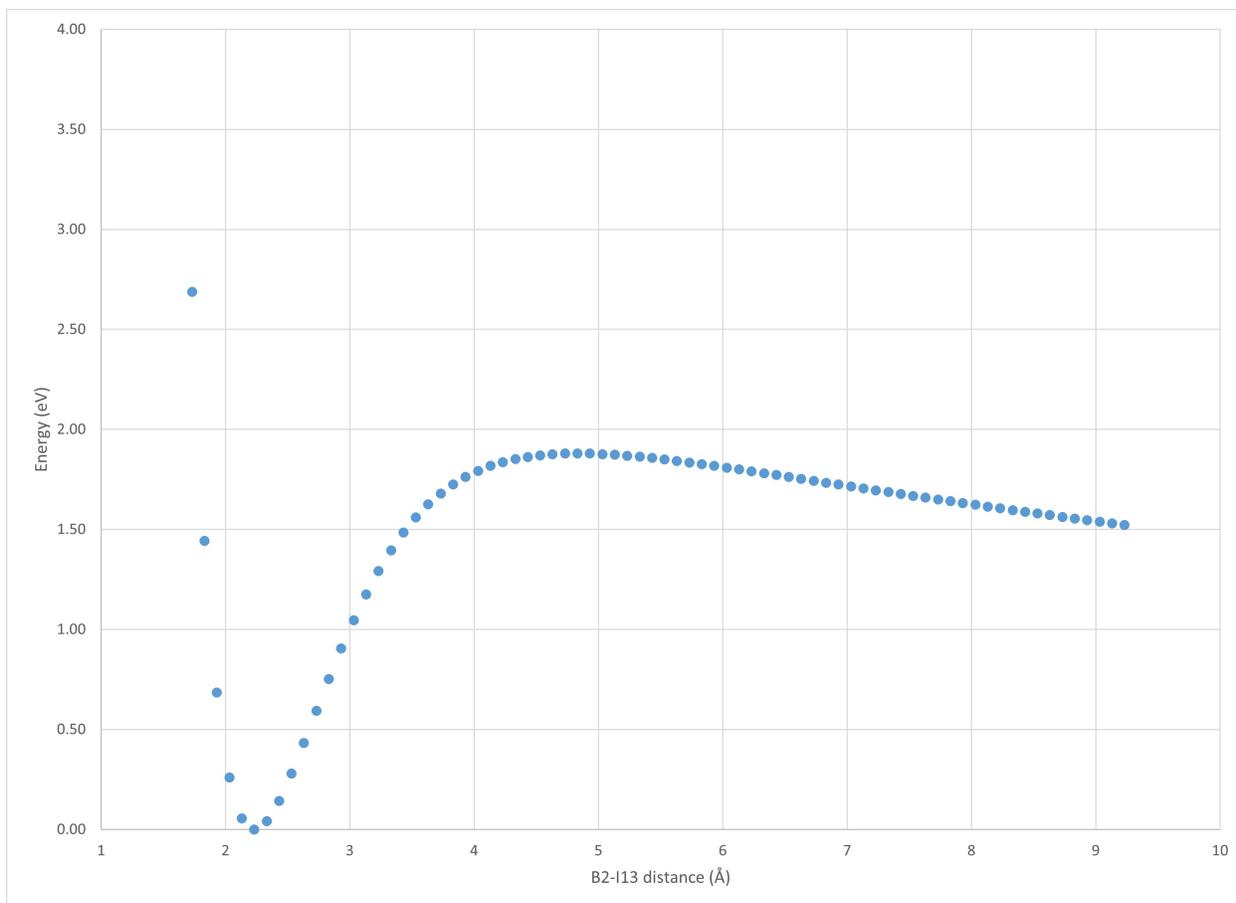
Figure S4: Plot of the relaxed scan of the B2-I13 distance in $[\text{B}_{12}\text{I}_{11}]^{2-\bullet}$ using the data in Table S23.

Table S26: Optimized geometry in Å for the transition state associated with the Coulomb barrier to break the B2-I13 bond in $[B_{12}I_{11}]^{2-\bullet}$.

Atom	x	y	z
B	-0.0003	0.0004	-0.0002
B	-0.0003	0.0007	1.5986
B	1.5267	0.0003	0.7997
B	1.2435	1.0064	-0.6639
B	-0.5128	1.5159	-0.6639
B	-1.2906	0.8173	0.7995
B	1.2446	1.0002	2.2708
B	2.0391	1.7183	0.8034
B	0.7679	2.6491	-0.0975
B	-0.8042	2.5428	0.8033
B	-0.5173	1.5114	2.2706
B	0.7667	2.6452	1.7064
I	-1.3145	-4.5469	2.6219
I	2.8861	-1.7612	0.7878
I	2.3112	0.6051	-2.5652
I	-1.6294	1.7478	-2.5652
I	-3.3814	0.0563	0.7876
I	2.3142	0.5985	4.1643
I	4.1686	2.3098	0.8030
I	1.2899	4.4495	-1.2682
I	-2.2868	4.1818	0.8027
I	-1.6361	1.7438	4.1640
I	1.2878	4.4429	2.8814

Table S27: Harmonic frequencies (cm^{-1}) and intensities (km mol6−1) for the transition state associated with the Coulomb barrier to break the B2-I13 bond in $[B_{12}I_{11}]^{2-\bullet}$.

Frequency	Intensity	Frequency	Intensity
-20.2173	3.0313	353.1506	27.9067
6.1346	0.4957	497.5936	93.8603
12.6183	0.4471	523.4528	3.5659
46.0438	0.0002	525.0312	0.1723
47.9674	0.0170	529.9520	0.0107
48.9218	0.0729	538.8186	0.0169
53.8704	0.0001	540.7100	33.3265
55.5138	0.0014	587.4724	1.1636
56.1613	0.0102	624.1093	0.6479
56.8905	0.0105	624.7174	3.3470
61.1548	0.1010	634.9428	0.0022
64.2701	0.0018	682.8573	0.0715
65.8610	0.0209	687.2539	1.7052
68.3794	0.0004	694.6424	0.0458
69.0489	0.0079	700.2072	0.0580
69.6428	0.0010	711.6210	64.3767
70.9160	0.0219	743.0919	5.0948
77.8012	0.5509	758.3250	2.0026
78.2611	0.6577	766.4784	7.0396
81.6902	0.0934	785.1204	0.0445
134.0132	4.8883	801.7051	0.2564
134.4985	0.1922	802.7656	8.5196
135.7259	0.0608	848.6256	27.1980
136.6680	0.0020	855.9309	20.4061
139.6208	0.1250	868.4359	352.8639
140.1393	0.0622	872.2796	145.0669
140.3579	0.0114	881.8181	16.2255
296.2375	25.4153	897.6706	251.0567
304.3188	7.6195	909.0105	0.4075
312.2140	19.7572	941.0672	186.4031
333.0829	2.8743	1069.5487	181.4616
341.5426	0.0058		

SIII.5 TS for the B–CN cleavage in $[B_{12}(CN)_{12}]^{2-}$

Table S28: Relaxed scan of the B1-C35 distance in $[B_{12}(CN)_{12}]^{2-}$. The energy is relative to the energy of the optimized species with a B1-C35 equilibrium bond length of 1.54 Å. The line in bold face corresponds to the geometry taken as a guess for the transition state optimization. The natural charge on C35 plus N36 was -0.66 e at a B1-C35 distance of 7.09 Å. The numbering of the atoms corresponds to the geometries given in Section SI.1.

B1-C35 dist. (Å)	Energy (eV)	B1-C35 dist. (Å)	Energy (eV)	B1-C35 dist. (Å)	Energy (eV)
0.54	105.3897	3.64	5.1432	5.69	5.8952
0.64	69.6616	3.74	5.2298	5.74	5.8912
0.74	43.4056	3.84	5.3068	5.79	5.8873
0.84	25.9968	3.94	5.3757	5.84	5.8835
0.94	15.0507	4.04	5.4365	5.89	5.8798
1.04	8.3237	4.14	5.4906	5.94	5.8761
1.14	4.2918	4.24	5.5384	5.99	5.8726
1.24	1.9683	4.34	5.5808	6.04	5.869
1.34	0.721	4.44	5.6174	6.09	5.8656
1.44	0.1499	4.54	5.6499	6.14	5.8622
1.54	0	**4.64**	**6.0155**	6.19	5.8588
1.64	0.1063	4.69	6.0075	6.24	5.8555
1.74	0.3644	4.74	5.9998	6.29	5.8522
1.84	0.7074	4.79	5.9925	6.34	5.8489
1.94	1.0906	4.84	5.9855	6.39	5.8457
2.04	1.4862	4.89	5.9787	6.44	5.8425
2.14	1.876	4.94	5.9722	6.49	5.8394
2.24	2.2494	4.99	5.9659	6.54	5.8363
2.34	2.6	5.04	5.9598	6.59	5.8332
2.44	2.9237	5.09	5.9539	6.64	6.0155
2.54	3.2232	5.14	5.9483	6.69	6.0155
2.64	3.4972	5.19	5.9429	6.74	6.0155
2.74	3.7467	5.24	5.9376	6.79	6.0155
2.84	3.9731	5.29	5.9325	6.84	6.0155
2.94	4.1793	5.34	5.9276	6.89	6.0155
3.04	4.3651	5.39	5.9228	6.94	6.0155
3.14	4.5321	5.44	5.9164	6.99	6.0155
3.24	4.6821	5.49	5.9119	7.04	6.0155
3.34	4.817	5.54	5.9076	7.09	6.0155
3.44	4.938	5.59	5.9033		
3.54	5.0464	5.64	5.8992		
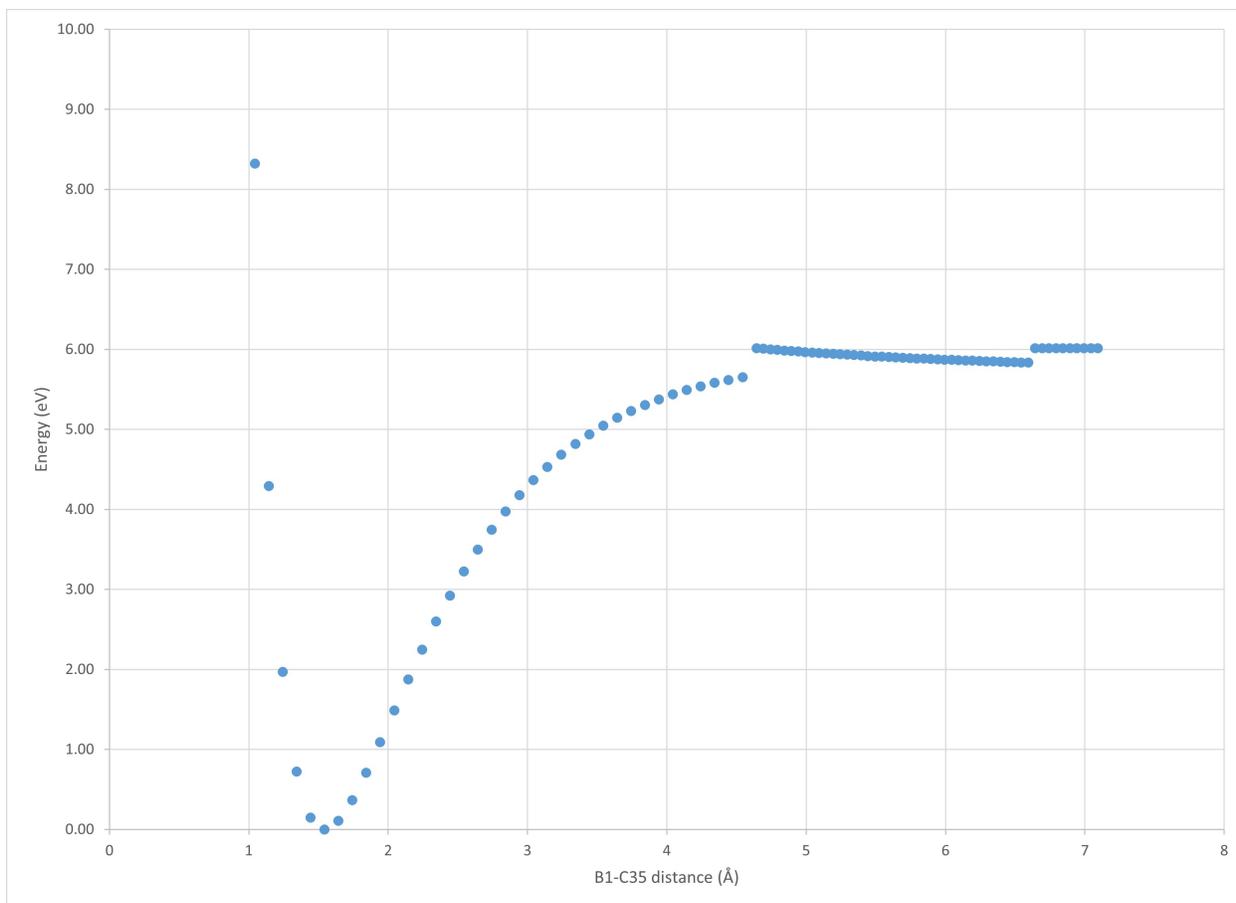
Figure S5: Plot of the relaxed scan of the B1-C35 distance in $[B_{12}(CN)_{12}]^{2-}$ using the data in Table S26.

Table S29: Optimized geometry in Å for the transition state associated with the Coulomb barrier to break the B1-C35 bond in $[B_{12}(CN)_{12}]^{2-}$.

Atom	x	y	z
B	1.2773	-0.0035	-0.0232
B	0.5364	0.3298	1.5081
B	0.5160	1.5446	0.1447
B	0.4850	0.6230	-1.4317
B	0.4865	-1.1612	-1.0425
B	0.5184	-1.3423	0.7744
B	-1.0024	1.1513	1.0401
B	-1.0338	1.3307	-0.7577
B	-1.0518	-0.3241	-1.4838
B	-1.0315	-1.5261	-0.1346
B	-1.0009	-0.6143	1.4252
B	-1.9548	0.0064	0.0344
C	1.2703	0.6183	2.8283
C	1.2320	2.9001	0.2673
C	1.1737	1.1692	-2.6936
C	1.1764	-2.1823	-1.9624
C	1.2361	-2.5225	1.4502
C	-1.6726	2.1814	1.9679
C	-1.7321	2.5214	-1.4401
C	-1.7664	-0.6153	-2.8164
C	-1.7278	-2.8937	-0.2588
C	-1.6699	-1.1654	2.6979
C	-3.4957	0.0112	0.0618
N	-2.2533	-3.9266	-0.3526
N	1.8111	0.8380	3.8335
N	1.6801	1.5850	-3.6537
N	1.7592	3.9317	0.3610
N	1.7646	-3.4208	1.9649
N	1.6836	-2.9594	-2.6623
N	-2.3055	-0.8352	-3.8227
N	-2.1747	-1.5815	3.6590
N	-4.6580	0.0149	0.0825
N	-2.2589	3.4207	-1.9554
N	-2.1783	2.9593	2.6685
C	7.3367	-0.0295	-0.1323
N	8.5167	-0.0352	-0.1538

Table S30: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition state associated with the Coulomb barrier to break the B1-C35 bond in $[B_{12}(CN)_{12}]^{2-}$.

Frequency	Intensity	Frequency	Intensity
-28.5520	16.3653	410.0467	0.0000
15.0917	7.0588	411.7051	0.0016
15.3128	7.0580	411.7237	0.0017
55.5114	0.0007	523.5121	316.0963
55.5553	0.0007	563.5283	2.0289
80.8716	0.0000	563.5672	2.0276
80.8991	0.0000	592.2002	0.0001
82.1337	0.0000	630.9416	0.1458
82.9515	0.0174	631.1748	1.6329
82.9748	0.0173	631.2676	0.8728
84.8379	0.0000	631.3687	0.8036
84.8715	0.0000	635.2315	20.1849
86.1228	0.0155	635.3434	20.0348
86.1531	0.0152	636.9255	0.0000
88.0172	0.0667	694.0895	7.4828
88.4063	0.0000	711.9702	0.0001
88.4136	0.0000	712.0031	0.0002
90.2592	0.0000	731.6971	0.0002
90.2733	0.0000	731.8699	0.0010
91.4303	0.0073	737.8986	0.0533
91.4486	0.0076	738.1042	0.0581
106.5819	21.2279	756.0679	0.0002
106.5961	21.2309	756.2628	0.0000
109.8519	25.7929	761.7800	0.1904
202.2340	0.3765	762.0376	0.1933
202.3923	0.3744	822.0367	37.7718
206.0412	0.0003	822.3679	12.1138
314.4316	0.1734	823.2567	130.1427
314.5344	0.1731	1078.9154	4.8190
324.6533	0.0026	1083.4007	0.0219
324.6942	0.0012	1084.0766	0.0101
335.8296	16.0883	1094.0491	14.1465
352.4249	0.3837	1094.3729	13.8063
353.5207	0.0002	1099.1656	97.4712
353.6740	0.0001	1104.6592	0.0040
360.0987	0.0003	1104.8316	0.0150
362.4989	2.5052	1112.7845	51.8064
362.5891	2.4836	1120.0600	110.6995
369.1965	0.0099	1120.2187	111.0006
369.2951	0.0287	2134.4091	112.7254
370.2674	18.7381	2336.3428	6.0184
379.5474	4.8217	2337.0376	0.2865
379.6188	4.8398	2337.0425	0.0499
390.5117	0.0002	2337.0628	4.3167
390.5391	0.0000	2337.0792	4.6200
396.0736	0.2203	2339.1225	0.3135
396.1048	0.2171	2340.7215	0.0023
404.8807	0.0001	2341.1241	6.8080
404.9147	0.0000	2341.1476	6.7952
408.2504	0.1568	2341.3926	0.0021
410.0412	0.0000	2341.4006	0.0139

SIII.6 TS for the B–CN cleavage in $[B_{12}(CN)_{11}]^{2-\bullet}$

Table S31: Relaxed scan of the B2-C13 distance in $[B_{12}(CN)_{11}]^{2-\bullet}$. The energy is relative to the energy of the optimized species with a B2-C13 equilibrium bond length of 1.55 Å. The line in bold face corresponds to the geometry taken as a guess for the transition state optimization. The natural charge on C13 plus N25 was -0.50 e at a B2-C13 distance of 3.35 Å. The numbering of the atoms corresponds to the geometries given in Section SI.1.

B1-C13 dist. (Å)	Energy (eV)
0.75	42.6093
0.85	25.5067
0.95	14.7584
1.05	8.1564
1.15	4.2018
1.25	1.9242
1.35	0.7046
1.45	0.1469
1.55	0.0000
1.65	0.1046
1.75	0.3557
1.85	0.6869
1.95	1.0548
2.05	1.4316
2.15	1.7990
2.25	2.1480
2.35	2.4717
2.45	2.7688
2.55	3.0382
2.65	3.2806
2.75	3.4969
2.85	3.6886
2.95	3.8568
3.05	4.0031
3.15	4.1291
3.25	4.2370
3.35	4.3291
3.45	4.4075
3.55	4.4745
3.65	4.5316
3.75	4.5802
3.85	**4.6216**
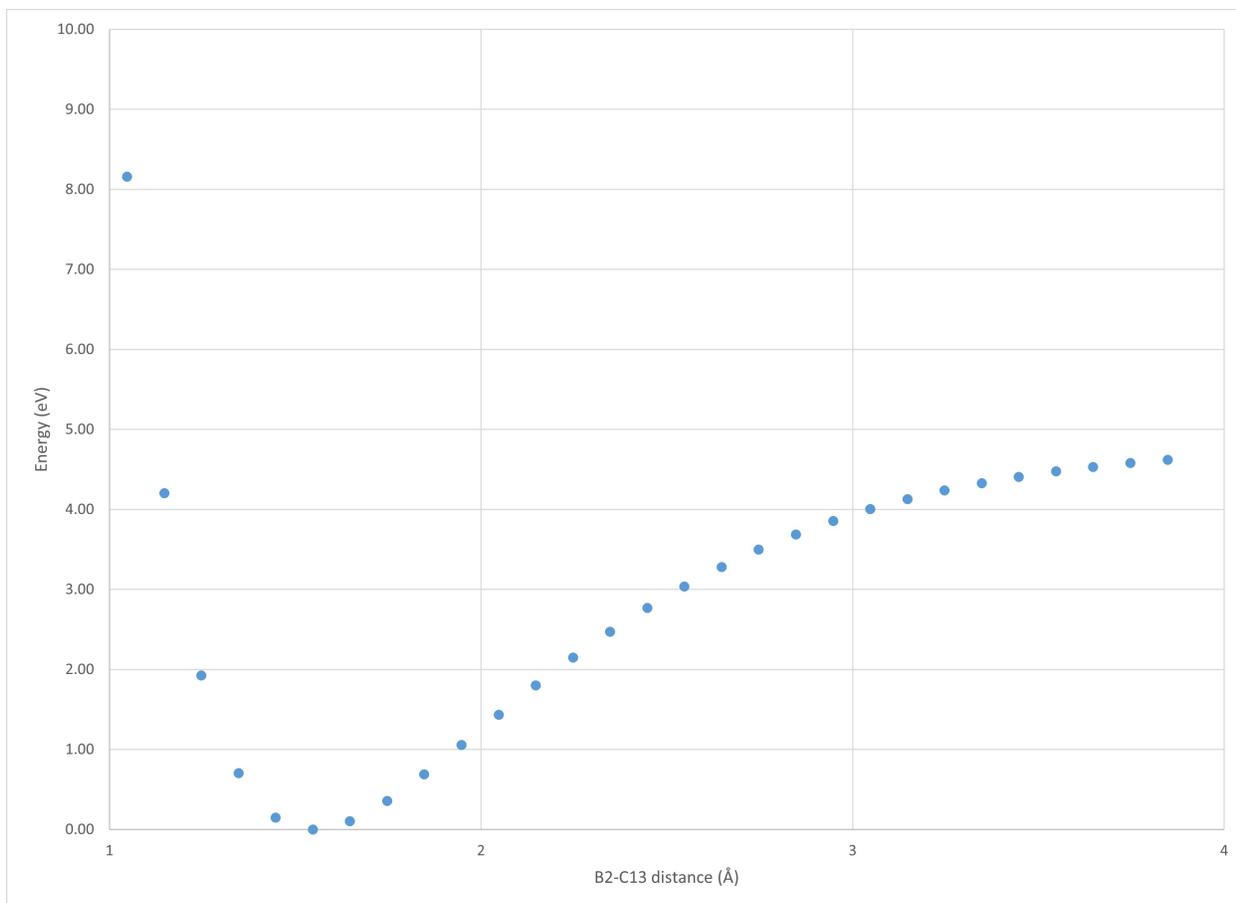
Figure S6: Plot of the relaxed scan of the B2-C13 distance in $[\text{B}_{12}(\text{CN})_{11}]^{2-\bullet}$ using the data in Table S29.

Table S32: Optimized geometry in Å for the transition state associated with the Coulomb barrier to break the B2-C13 bond in $[B_{12}(CN)_{11}]^{2-\bullet}$.

Atom	x	y	z
B	0.7235	-0.0027	-1.3393
B	1.5298	-0.0012	0.0310
B	0.7290	1.4754	-0.4223
B	-0.7710	0.9123	-1.2455
B	-0.7725	-0.9149	-1.2427
B	0.7265	-1.4779	-0.4177
B	0.7181	0.9148	1.2891
B	-0.8205	1.4741	0.4879
B	-1.7311	0.0015	-0.0169
B	-0.8230	-1.4711	0.4925
B	0.7165	-0.9119	1.2920
B	-0.8214	0.0031	1.5314
C	5.7117	-0.0109	-3.7257
C	1.4506	2.7782	-0.8455
C	-1.4385	1.6993	-2.3933
C	-1.4414	-1.7043	-2.3880
C	1.4459	-2.7832	-0.8368
C	1.3969	1.7037	2.4291
C	-1.5423	2.7697	0.9108
C	-3.2726	0.0027	-0.0566
C	-1.5469	-2.7641	0.9195
C	1.3940	-1.6983	2.4345
C	-1.5368	0.0059	2.8975
N	-2.0841	-3.7456	1.2368
N	6.7010	-0.0128	-4.3652
N	-1.9301	2.2944	-3.2631
N	1.9867	3.7618	-1.1575
N	1.9804	-3.7687	-1.1457
N	-1.9340	-2.3013	-3.2559
N	-4.4350	0.0037	-0.0883
N	1.9163	-2.2923	3.2870
N	-2.0739	0.0080	3.9288
N	-2.0777	3.7531	1.2250
N	1.9202	2.2995	3.2797

Table S33: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition state associated with the Coulomb barrier to break the B2-C13 bond in $[\text{B}_{12}(\text{CN})_{11}]^{2-\bullet}$.

Frequency	Intensity	Frequency	Intensity
-28.1305	7.1699	415.0437	0.1515
5.1961	3.8014	467.8032	51.9499
17.8182	4.2536	517.0008	94.9476
53.9116	0.9438	534.4018	2.0210
61.1514	0.5755	556.3179	1.8553
80.6903	0.0000	581.6109	0.0006
82.6518	0.0402	624.8368	3.0806
82.8761	0.0143	628.0656	16.6272
83.3924	0.0000	631.8249	0.0496
84.2738	0.0495	632.7560	3.0811
84.8696	0.0252	632.8180	0.0043
86.2690	0.0954	639.4902	0.0009
86.3515	0.1995	660.2439	51.6411
87.8686	0.0002	702.6240	6.3297
89.9126	0.0048	716.6408	0.0008
91.1885	0.0000	722.3642	1.1227
91.3337	0.0439	736.9005	0.0398
91.6733	0.0306	745.8114	1.9858
91.8731	0.0282	751.9422	0.5579
105.0956	16.6027	755.6372	0.0491
105.0962	16.6006	756.1483	0.0031
110.7368	22.6366	763.7439	0.0653
200.5465	1.7743	786.9483	25.5085
202.3711	2.0680	793.9050	2.7555
205.6140	0.0004	829.5205	0.0002
324.8326	0.1277	830.2834	0.1135
324.8789	0.1666	1034.6819	137.6108
328.7436	0.0000	1069.0721	0.3769
330.2624	1.8513	1074.1082	168.8709
340.0273	0.5214	1077.3258	25.7588
351.2346	0.9355	1083.0673	0.1242
353.4305	2.9483	1086.0365	240.2602
364.3755	2.0228	1088.4504	0.0060
364.4257	0.0208	1096.9615	155.0566
365.8952	1.6608	1103.5298	74.5450
368.3544	11.1460	1110.4032	174.6393
373.6962	5.3004	1119.9132	76.6562
374.6153	0.0003	2138.4092	263.1427
386.4512	6.1321	2332.2083	2.6007
387.4955	0.7076	2332.8386	0.5052
395.3442	0.0098	2333.5323	1.2523
397.7074	1.4400	2333.7252	1.9962
402.6406	0.0108	2333.9588	0.2072
403.9096	0.0001	2333.9953	0.0331
410.3062	0.0592	2334.2283	1.6406
411.5039	0.0607	2334.4586	0.0272
412.6459	0.0000	2335.2177	0.2095
414.4881	0.0033	2335.3929	0.0008

SIV Pathway energies, intermediates, and transition states

SIV.1 Geometries, TS frequencies, and Gibbs energies for species in Figure 4 of the main text

Table S34: Optimized geometry in Å for the species in Figure 4 of the main text.

I				TS1			
Atom	x	y	z	Atom	x	y	z
B	0.112325	0.846979	-1.673243	B	-0.03315	-0.914603	-1.698747
B	-0.112497	-0.847128	-1.673215	B	-0.025056	0.833602	-1.740309
B	1.423518	-0.1775	-1.191225	B	-1.461493	-0.005793	-1.174489
B	1.073644	1.307358	-0.28843	B	-0.904104	-1.438173	-0.273978
B	-0.698209	1.52921	-0.302124	B	0.893544	-1.459089	-0.304539
B	-1.423742	0.17739	-1.190961	B	1.427405	-0.035602	-1.241397
B	0.698155	-1.529367	-0.302239	B	-0.890478	1.455291	-0.331125
B	1.4546	-0.191806	0.590932	B	-1.448996	0.026225	0.599282
B	0.115642	0.889859	1.153705	B	0.018573	-0.878424	1.144843
B	-1.454515	0.191705	0.591139	B	1.474983	0.006607	0.543427
B	-1.07363	-1.307501	-0.288235	B	0.904916	1.439473	-0.370126
B	-0.115472	-0.890002	1.153742	B	0.028597	0.924025	1.109174
Br	3.039242	-0.330236	-2.392613	Br	-3.077155	0.002359	-2.315127
Br	2.300145	2.878107	-0.394148	Br	-1.921647	-3.124127	-0.394518
Br	-1.453304	3.373863	-0.524407	Br	1.893458	-3.145799	-0.356255
Br	-3.039572	0.330707	-2.392101	Br	3.004308	-0.044861	-2.424988
Br	1.453328	-3.373962	-0.524537	Br	-1.898289	3.135527	-0.416651
Br	3.128444	-0.425224	1.59809	Br	-3.111075	0.041141	1.629276
Br	0.244017	1.953876	2.799247	Br	0.028768	-1.900495	2.810328
Br	-3.128127	0.42512	1.598215	Br	3.166714	0.016281	1.523078
Br	-2.300329	-2.878074	-0.39428	Br	1.925443	3.108874	-0.490729
Br	-0.243823	-1.953914	2.79923	Br	0.064962	1.9948	2.742841
O	0.220359	1.789851	-2.952332	O	-0.101317	-1.785589	-2.942336
H	-0.192286	2.652666	-2.688805	H	-0.762179	-2.515535	-2.836605
H	1.167073	1.949752	-3.166006	H	-0.235224	-1.286566	-3.830908
O	-0.220457	-1.790288	-2.952068	O	-0.063874	1.58626	-3.075663
H	-1.167036	-1.951463	-3.165119	H	0.667827	1.293278	-3.690317
H	0.193215	-2.652619	-2.688411	H	-0.914681	1.406238	-3.562139

Table S35: Optimized geometry in Å for the species in Figure 4 of the main text.

II				TS2			
Atom	x	y	z	Atom	x	y	z
B	-0.040318	0.938784	-1.827578	B	-0.000168	-1.032736	-1.882005
B	-0.040315	-0.93879	-1.827578	B	-0.000056	1.032725	-1.881897
B	1.445559	0.000005	-1.281187	B	-1.512587	-0.000031	-1.238765
B	0.9171	1.442767	-0.390292	B	-0.938628	-1.449789	-0.382582
B	-0.92352	1.441784	-0.323085	B	0.938619	-1.449754	-0.382536
B	-1.457438	-0.000002	-1.210925	B	1.512706	-0.00026	-1.238525
B	0.917107	-1.442764	-0.390293	B	-0.938419	1.44988	-0.382238
B	1.47713	0.000003	0.500289	B	-1.45272	0.000195	0.542354
B	0.028872	0.909923	1.086236	B	-0.000054	-0.933209	1.043743
B	-1.462786	-0.000006	0.556404	B	1.452725	-0.000053	0.542713
B	-0.923514	-1.441789	-0.32309	B	0.938752	1.449586	-0.382214
B	0.028871	-0.909925	1.086235	B	0.000075	0.933019	1.043972
Br	3.049545	0.00001	-2.388335	Br	-3.093299	0.000282	-2.338304
Br	1.917868	3.111712	-0.444862	Br	-1.940435	-3.118058	-0.386294
Br	-1.941286	3.10439	-0.370019	Br	1.939898	-3.118368	-0.386208
Br	-3.065586	0.00001	-2.356348	Br	3.093503	-0.000112	-2.337963
Br	1.917882	-3.111704	-0.444866	Br	-1.939788	3.118393	-0.386394
Br	3.155684	0.000005	1.50156	Br	-3.110839	0.00027	1.550694
Br	0.055567	1.934785	2.733628	Br	-0.000376	-1.942833	2.703215
Br	-3.113975	-0.000011	1.599063	Br	3.110764	-0.00021	1.551133
Br	-1.941277	-3.104401	-0.370031	Br	1.940264	3.118035	-0.386181
Br	0.055572	-1.934791	2.733624	Br	-0.000084	1.942701	2.703441
O	-0.065993	1.631696	-3.018709	O	-0.000164	-1.582243	-3.04492
H	-0.963914	1.710298	-3.372921	H	0.0044	-0.409425	-4.170897
O	-0.065976	-1.631702	-3.01871	O	0.000719	1.582201	-3.044697
H	-0.963905	-1.710412	-3.372876	H	0.003664	0.40836	-4.172121

Table S36: Optimized geometry in Å for the species in Figure 4 of the main text.

III				TS3			
Atom	x	y	z	Atom	x	y	z
B	0.000011	-1.25761	-1.943628	B	0.000001	-0.832007	-1.850541
B	0.000011	1.25761	-1.943628	B	-0.000001	0.863883	-1.841559
B	-1.605182	0	-1.230968	B	-1.493169	0.024194	-1.218887
B	-0.967055	-1.430907	-0.421389	B	-0.889465	-1.483542	-0.41482
B	0.967058	-1.430922	-0.421458	B	0.889466	-1.483541	-0.41482
B	1.605331	0	-1.231015	B	1.49317	0.024196	-1.218886
B	-0.967055	1.430907	-0.421389	B	-0.88986	1.492016	-0.417334
B	-1.450912	0	0.530917	B	-1.47687	-0.015469	0.500665
B	0.000047	-0.929709	1.004122	B	0.000001	-0.900824	1.053843
B	1.45089	0	0.530947	B	1.47687	-0.015468	0.500666
B	0.967058	1.430922	-0.421458	B	0.889859	1.492017	-0.417334
B	0.000047	0.929709	1.004122	B	-0.000001	0.891282	1.056871
Br	-3.151039	0	-2.345898	Br	-3.106105	0.021985	-2.302139
Br	-1.944175	-3.11775	-0.400822	Br	-1.909154	-3.138919	-0.463299
Br	1.944119	-3.117779	-0.400859	Br	1.909158	-3.138918	-0.463298
Br	3.15107	0	-2.345902	Br	3.106106	0.021989	-2.302138
Br	-1.944175	3.11775	-0.400823	Br	-1.913743	3.148211	-0.41714
Br	-3.103731	0	1.551975	Br	-3.111186	-0.021193	1.551901
Br	0.000019	-1.942942	2.663354	Br	0.000001	-1.932664	2.706487
Br	3.103708	0	1.552058	Br	3.111185	-0.021189	1.551903
Br	1.944119	3.117779	-0.40086	Br	1.91374	3.148213	-0.417141
Br	0.000019	1.942942	2.663354	Br	-0.000001	1.899185	2.715326
O	0.000066	-1.647788	-3.120068	O	0.000003	-0.928976	-3.255498
O	0.000066	1.647788	-3.120068	O	0	0.951702	-3.270187

Table S37: Optimized geometry in Å for the species in Figure 4 of the main text.

IV				TS4			
Atom	x	y	z	Atom	x	y	z
B	-0.000062	0.840155	-1.813528	B	-0.08961	-1.271833	1.226416
B	-0.000057	-0.84007	-1.813661	B	-0.078479	0.252071	1.760922
B	1.483218	0.000038	-1.216491	B	1.408445	-0.410747	1.181348
B	0.89021	1.497903	-0.414618	B	0.896799	-1.486503	-0.175637
B	-0.890231	1.49791	-0.414616	B	-0.934515	-1.439483	-0.271118
B	-1.483236	0.000025	-1.216467	B	-1.52884	-0.335813	1.027626
B	0.890208	-1.497917	-0.41476	B	0.917201	1.284326	0.800518
B	1.475962	-0.000043	0.497949	B	1.515904	0.181501	-0.502857
B	-0.00001	0.896643	1.05246	B	0.068106	-0.447657	-1.386807
B	-1.475959	-0.000034	0.497982	B	-1.429557	0.257287	-0.656747
B	-0.890217	-1.497903	-0.414716	B	-0.914497	1.331488	0.704897
B	0.000024	-0.896785	1.052378	B	0.080644	1.24562	-0.790398
Br	3.094346	0.000161	-2.317501	Br	2.90975	-0.843013	2.374463
Br	1.920678	3.149009	-0.431616	Br	1.885061	-3.115017	-0.610758
Br	-1.920729	3.149009	-0.431558	Br	-1.956138	-3.013742	-0.815071
Br	-3.094358	0.000104	-2.317501	Br	-3.16688	-0.687188	2.055519
Br	1.920757	-3.148981	-0.431839	Br	1.932425	2.809741	1.479406
Br	3.113615	-0.000069	1.547849	Br	3.238905	0.472273	-1.367817
Br	0.00004	1.91217	2.712474	Br	0.156741	-0.874331	-3.290098
Br	-3.113597	-0.000075	1.547902	Br	-3.035397	0.63458	-1.696397
Br	-1.920754	-3.148975	-0.431792	Br	-1.9161	2.908163	1.278758
Br	0.000039	-1.912409	2.712333	Br	0.183719	2.767358	-2.009723
O	-0.000056	0.730706	-3.279088	O	-0.287494	-2.353392	4.286717
O	-0.000014	-0.730406	-3.27915	O	-0.672634	-1.754121	5.271944

Table S38: Optimized geometry in Å for the species in Figure 4 of the main text.

VI			
Atom	x	y	z
B	-0.007716	0.63186	-1.723445
B	-0.012205	-1.09846	-1.804334
B	1.474303	-0.11687	-1.313532
B	0.917315	1.441209	-0.532496
B	-0.910487	1.455736	-0.515519
B	-1.489232	-0.086428	-1.291306
B	0.900422	-1.452474	-0.280729
B	1.465633	0.071448	0.479802
B	0.00905	1.026273	0.966596
B	-1.462595	0.084587	0.492104
B	-0.902992	-1.438835	-0.281472
B	0.003263	-0.766268	1.106342
Br	3.050341	-0.185623	-2.459341
Br	1.914733	3.093481	-0.826157
Br	-1.894645	3.118199	-0.794922
Br	-3.071899	-0.15652	-2.429936
Br	1.9094	-3.123768	-0.178802
Br	3.142512	0.167158	1.471469
Br	0.02325	2.216726	2.51155
Br	-3.129379	0.180624	1.501213
Br	-1.922114	-3.112604	-0.216977
Br	-0.000707	-1.653043	2.846402
O	-0.027333	-1.885631	-2.947843
H	-0.4574	-2.735925	-2.784748

Table S39: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition states in Figure 4 of the main text.

TS1				TS2			
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
-234.9017	87.8044	564.9092	1.7557	-800.595	520.6806	467.7402	2.4605
67.3383	0.1999	565.9088	0.1983	70.7723	0.0151	469.8268	31.8479
69.8847	0.3144	567.7077	1.1248	71.2055	0	521.5607	0.1788
71.745	0.022	574.7977	0.4115	74.9613	0.0243	523.5621	21.7645
80.0224	0.092	626.9375	15.7033	80.3299	0.1739	535.5237	0.0004
80.9888	0.0888	663.9713	0.5583	82.5006	0	566.8303	24.3846
82.209	0.007	669.4072	0.6094	86.1426	0.0135	580.7127	10.9411
84.06	0.0421	672.5251	0.251	89.0332	0.0083	583.3613	0.0001
88.5943	0.3132	688.066	2.7665	93.8391	0.0614	596.3516	0.5781
91.8288	0.1753	707.0933	2.5808	95.6087	0	636.1187	0.0005
92.941	0.0713	710.6306	50.484	96.5886	0.0106	644.608	0.3558
97.1433	0.0915	723.4123	0.8419	101.9237	0.0006	646.2017	28.9103
97.9938	0.0201	724.3754	1.4814	102.2888	0.0026	675.9339	4.3118
98.7981	0.006	731.806	4.7128	102.9977	0.0115	680.2776	50.0977
100.5367	0.0116	739.3396	19.1707	103.1477	0	707.9896	0.294
101.6498	0.0081	769.0623	1.8247	107.19	0.0008	710.6959	9.4618
103.2574	0.1268	776.994	1.5005	107.2098	0.2062	722.9631	0
108.3416	0.3408	789.8002	3.6184	111.3653	0.0279	762.7371	43.3298
139.0585	6.2756	807.7838	35.459	129.9661	0.2649	857.0743	0.0003
160.5958	2.6495	874.0976	0.6851	165.8074	1.0139	857.8894	0.6031
179.6642	8.1248	877.7322	1.1065	180.2483	0.0003	867.0774	0.1502
184.0576	2.546	888.9032	36.8185	185.3108	2.001	870.0837	67.3427
188.8641	4.2716	912.8148	30.7981	185.6445	0.094	882.6463	42.8968
191.9741	0.1785	924.7255	42.7575	186.1839	0.0913	904.3978	69.1731
192.6452	0.0799	933.3104	87.4998	189.0979	0.0363	914.0844	0.0092
195.6106	0.9963	942.1174	16.5301	200.3931	0.027	940.6145	237.2515
199.9472	0.0201	947.1022	274.8012	205.9091	0.0366	945.8257	235.6611
201.5529	0.0632	952.1735	216.9993	210.4139	0.0001	953.6141	417.3252
204.4496	0.0917	963.71	232.1976	238.8592	5.1416	962.6616	0.5704
306.5665	17.3123	967.6438	71.2542	287.8313	0.4142	970.4747	9.3653
330.2436	11.7834	1004.8293	46.0959	310.1818	3.1226	1442.2729	0.7537
349.7694	1.0683	1027.7439	22.8467	379.9861	9.5196	1480.6051	59.8359
389.2436	0.1156	1035.239	85.9233	384.5747	3.2302	3062.1287	760.0655
395.4688	3.0194	1440.6614	119.9594	385.6743	4.7991		
402.5792	1.11	1516.4132	148.8945	392.6112	0		
435.5619	37.7983	2432.1101	1810.3446	419.1246	12.6397		
481.3038	53.2313	3145.5044	320.9065	428.2571	15.619		
520.4565	3.7119	3236.1531	490.1086	445.5013	0.0109		
562.5137	1.0323	3385.9656	75.5064	462.2307	55.4198		

Table S40: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition states in Figure 4 of the main text.

TS3				TS4			
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
-669.5919	22.4564	541.3651	15.9998	-17.7875	0.0059	552.168	10.5374
64.483	0.006	557.1071	13.9748	13.6652	0.005	553.935	0.0217
71.7059	0.001	558.7119	2.4879	28.9315	0.0281	615.1406	14.3955
75.2032	0.0017	590.0845	5.9605	38.195	0.0354	650.7937	1.7763
78.362	0.0139	610.3388	4.5308	66.5405	0.0001	652.8851	0.0017
81.9331	0.0003	649.8238	15.3216	69.2831	0.0193	661.6502	3.9352
81.9602	0.0211	661.4953	1.7038	70.6904	0.0072	699.6224	0.0449
90.2027	0.0283	666.2765	1.5137	73.4994	0.1367	700.0458	0.0356
90.8308	0.0178	674.421	2.0748	79.2617	0.0001	705.5778	0.0238
94.6484	0.0003	684.779	22.3398	81.217	0.0011	707.6229	0.7867
96.9375	0.0005	709.5853	12.5738	81.5552	0.0004	725.7221	5.6571
100.3772	0.0083	720.8593	23.9913	84.2864	0.007	747.5093	66.6114
102.9968	0.0072	725.5263	42.8927	88.0985	0.0349	773.0014	21.4177
103.2673	0.0003	747.1455	42.3626	90.6126	0	782.2736	2.5659
103.5335	0.0062	847.4624	66.1616	92.1444	0.0028	802.1271	0.0153
105.5399	0.1376	859.9417	13.9392	100.0143	0.0005	871.9256	34.0018
109.2514	0.1489	867.5007	6.7728	100.6234	0.0001	886.6324	0.025
110.4269	0.0751	878.6072	58.5317	101.0888	0.001	905.0613	5.5372
153.776	0.6512	886.8927	8.4087	101.5102	0.0006	909.8189	1.4099
172.9146	0.0272	902.3778	60.4282	105.9877	0.0322	932.165	100.6845
176.3862	0.0914	929.0272	243.5598	106.6355	0.051	943.937	121.399
184.4673	0.1042	946.9587	205.3842	109.9518	0.0012	949.5035	0.1357
188.2715	0.0107	948.2225	49.5774	185.5618	0.0347	955.8573	41.125
192.1536	0.1356	984.0653	312.5764	188.9041	0.0146	959.3226	253.3131
195.1563	1.18	984.2104	1.7582	191.7051	0.0032	981.0385	164.5154
200.2961	0.0199	1017.3343	10.0008	192.6208	0	1072.6821	0.0135
203.4428	0.0008	1128.7406	22.7327	199.5963	0.0198	1629.0253	13.3109
241.2077	0.0428			202.4036	0.0024		
297.1393	0.5256			206.5476	0.0134		
365.5396	7.677			332.2124	3.3184		
373.6587	0.0004			334.5421	3.6693		
405.4903	2.0232			361.2691	0.0082		
418.0234	2.9678			367.0315	13.3165		
448.9338	43.2549			378.8051	0.6705		
463.4048	25.4072			426.6775	37.3967		
508.285	0.2106			513.3584	114.8104		
523.1063	0.6436			539.2165	0.1643		
526.8505	33.9319			544.117	0.0315		
529.9927	0.0949			545.8333	1.9988		

Table S41: Calculated Gibbs energy (G), Gibbs energy within the pathway (G pathway), and relative Gibbs energy for the species shown in Figure 4 of the main text at 298.15 K.

Species	G (E_h)	G pathway (E_h)	Rel. G (eV)
I	-26169.05477	-26169.05477	0
TS1	-26169.05249	-26169.05249	0.06
II	-26167.96235	-	-
H_2	-1.179849	-	-
II + H_2	-26169.1422	-26169.1422	-2.38
TS2	-26167.81124	-	-
TS2 + H_2	-26168.99109	-26168.99109	1.73
III	-26166.66177	-	-
III + 2 H_2	-26169.02147	-26169.02147	0.91
TS3	-26166.58039	-	-
TS3 + 2 H_2	-26168.94009	-26168.94009	3.12
IV	-26166.60048	-	-
IV + 2 H_2	-26168.96017	-26168.96017	2.57
TS4	-26166.50136	-	-
TS4 + 2 H_2	-26168.86106	-26168.86106	5.27
V	-26016.16489	-	-
O_2	-150.343819	-	-
V + 2 H_2 + O_2	-26168.8684	-26168.8684	5.07

Table S42: Calculated Gibbs energy (G), Gibbs energy within the pathway (G pathway), and relative Gibbs energy for the species shown in Figure 4 of the main text at 298.15 K.

Species	G (E_h)	G pathway (E_h)	Rel. G (eV)
I	-26169.05477	-26169.05477	0
TS1	-26169.05249	-26169.05249	0.06
II	-26167.96235	-	-
H_2	-1.179849	-	-
II + H_2	-26169.1422	-26169.1422	-2.38
VI	-26092.06938	-	-
OH	-75.747516	-	-
VI + H_2 + OH	-26168.99675	-26168.99675	1.58
V	-26016.16489	-	-
V + H_2 + 2 OH	-26168.83977	-26168.83977	5.85

SIV.2 Geometries, TS frequencies, and Gibbs energies for species in Figure 5 of the main text

Table S43: Optimized geometry in Å for the species in Figure 5 of the main text.

VII				TS5			
Atom	x	y	z	Atom	x	y	z
B	0.066854	0.863417	-1.726182	B	0.024146	-0.907669	-1.774717
B	-0.066094	-0.862958	-1.726321	B	-0.009353	0.873738	-1.857342
B	1.430496	-0.101085	-1.242531	B	-1.44132	-0.060037	-1.288445
B	0.998773	1.360741	-0.334322	B	-0.877223	-1.48089	-0.361098
B	-0.782204	1.485929	-0.345044	B	0.931986	-1.427713	-0.364615
B	-1.430115	0.100794	-1.243269	B	1.450669	0.030731	-1.275757
B	0.782341	-1.486232	-0.345096	B	-0.928025	1.428586	-0.436978
B	1.462591	-0.110553	0.544124	B	-1.467048	-0.015955	0.493596
B	0.066237	0.895105	1.11323	B	0.015643	-0.878295	1.075747
B	-1.462762	0.110241	0.543568	B	1.462947	0.05146	0.505251
B	-0.998588	-1.361173	-0.33512	B	0.876583	1.4806	-0.419344
B	-0.066549	-0.895532	1.112786	B	-0.024052	0.930604	1.036854
I	3.204552	-0.185892	-2.6929	I	-3.186889	-0.119552	-2.651246
I	2.292258	3.208774	-0.541798	I	-1.973206	-3.390748	-0.441901
I	-1.775328	3.512214	-0.638814	I	2.104472	-3.298592	-0.513535
I	-3.203633	0.187555	-2.693423	I	3.204361	-0.00151	-2.630199
I	1.775695	-3.512424	-0.639491	I	-2.115293	3.282723	-0.619134
I	3.378906	-0.264287	1.658405	I	-3.366208	-0.029073	1.606297
I	0.149126	2.10963	2.967869	I	0.044239	-2.024162	2.953068
I	-3.379387	0.263571	1.65724	I	3.354771	0.095313	1.629568
I	-2.292308	-3.208674	-0.543298	I	1.983507	3.379726	-0.547558
I	-0.150309	-2.110431	2.967287	I	-0.064686	2.1406	2.873487
O	0.130908	1.776955	-2.988706	O	0.069517	-1.620455	-3.075522
H	-0.46385	2.553748	-2.816367	H	0.901255	-2.13105	-3.16662
H	1.048106	2.120064	-3.090049	H	0.052405	-0.82507	-3.89069
O	-0.129187	-1.776443	-2.989029	O	0.001246	1.485337	-3.150654
H	-1.04613	-2.120112	-3.091189	H	-0.851826	1.904261	-3.355054
H	0.465893	-2.55313	-2.816646	H	0.048708	0.16662	-4.362834

Table S44: Optimized geometry in Å for the species in Figure 5 of the main text.

VIII				TS6			
Atom	x	y	z	Atom	x	y	z
B	-0.032164	0.915494	-1.944031	B	0.000056	1.049177	-1.960455
B	0.032208	-0.915523	-1.944001	B	-0.000043	-1.049202	-1.960419
B	1.425767	0.038942	-1.358929	B	1.523789	-0.000049	-1.314033
B	0.839752	1.468319	-0.470681	B	0.946544	1.452616	-0.457585
B	-0.930378	1.412701	-0.45261	B	-0.946568	1.452585	-0.457619
B	-1.425728	-0.038994	-1.358947	B	-1.523797	-0.000078	-1.314005
B	0.930384	-1.412724	-0.452546	B	0.946559	-1.452603	-0.457607
B	1.445433	0.046532	0.426748	B	1.458077	0.000047	0.471329
B	-0.02786	0.894106	0.99446	B	-0.00002	0.932404	0.972895
B	-1.445417	-0.046526	0.426749	B	-1.45807	0.000014	0.471352
B	-0.83974	-1.468324	-0.470616	B	-0.946552	-1.452618	-0.457618
B	0.027862	-0.894056	0.994506	B	0.00001	-0.932369	0.972897
I	3.248115	0.066519	-2.617888	I	3.252138	-0.000032	-2.621446
I	1.928017	3.392454	-0.513897	I	2.067476	3.337801	-0.501276
I	-2.128595	3.27199	-0.505851	I	-2.067525	3.337757	-0.50131
I	-3.24808	-0.066656	-2.617898	I	-3.252108	-0.000065	-2.621466
I	2.128571	-3.27204	-0.505737	I	2.067516	-3.337786	-0.501204
I	3.333255	0.110607	1.576583	I	3.331684	0.000067	1.605475
I	-0.064194	2.06335	2.867759	I	-0.000021	2.096365	2.829939
I	-3.33326	-0.110529	1.576555	I	-3.331682	0.000041	1.60549
I	-1.92803	-3.392444	-0.51379	I	-2.067491	-3.337815	-0.501189
I	0.064178	-2.063223	2.867852	I	0.000019	-2.096318	2.829929
O	-0.01244	1.645722	-3.136747	O	-0.000074	1.58521	-3.126783
H	-0.827038	1.540498	-3.64437	H	0.000008	0.406675	-4.266552
O	0.012427	-1.645692	-3.136764	O	0.000031	-1.585244	-3.126756
H	0.827763	-1.541961	-3.643512	H	0.000045	-0.406748	-4.266692

Table S45: Optimized geometry in Å for the species in Figure 5 of the main text.

IX				TS7			
Atom	x	y	z	Atom	x	y	z
B	-0.02329	-0.949342	-1.97916	B	-0.000072	0.861289	-1.940629
B	0.02328	0.949404	-1.97913	B	0.00022	-0.85179	-1.94485
B	-1.455155	-0.048493	-1.373084	B	1.471608	0.004011	-1.325736
B	-0.904579	-1.450648	-0.446825	B	0.906632	1.461869	-0.515815
B	0.894174	-1.430885	-0.510168	B	-0.907732	1.461002	-0.515937
B	1.455149	0.048535	-1.37309	B	-1.471595	0.002814	-1.325747
B	-0.894177	1.4309	-0.510119	B	0.906772	-1.457463	-0.522178
B	-1.448463	-0.008162	0.41752	B	1.46069	0.000125	0.418121
B	0.001184	-0.903432	0.971881	B	-0.000349	0.900388	0.925357
B	1.448465	0.008148	0.417513	B	-1.460696	-0.000984	0.418189
B	0.904577	1.450662	-0.446785	B	-0.905932	-1.458147	-0.522054
B	-0.001179	0.903402	0.971909	B	0.000357	-0.90484	0.921795
I	-3.296484	-0.036764	-2.579421	I	3.293862	0.006031	-2.573786
I	-2.019438	-3.35261	-0.500143	I	2.079105	3.334119	-0.521428
I	2.053674	-3.30925	-0.571039	I	-2.081642	3.332409	-0.521114
I	3.296472	0.036844	-2.579435	I	-3.293893	0.004512	-2.5737
I	-2.053676	3.309268	-0.570927	I	2.079998	-3.327463	-0.534104
I	-3.331597	0.015075	1.562234	I	3.317925	-0.003725	1.610492
I	0.02881	-2.078056	2.834208	I	-0.000778	2.054399	2.81022
I	3.331604	-0.015123	1.562218	I	-3.31796	-0.006184	1.610502
I	2.019435	3.352625	-0.500048	I	-2.077401	-3.329213	-0.534543
I	-0.028797	2.077968	2.834272	I	0.000807	-2.069444	2.803674
O	-0.006931	-1.652436	-3.11715	O	-0.000362	0.963257	-3.366053
O	0.006916	1.652533	-3.117099	O	0.000263	-0.944482	-3.370427

Table S46: Optimized geometry in Å for the species in Figure 5 of the main text.

X				TS8			
Atom	x	y	z	Atom	x	y	z
B	-0.000043	0.845521	-1.911889	B	0.070881	-0.79558	1.634342
B	0.000031	-0.845519	-1.912166	B	0.072058	0.817831	1.622918
B	1.463196	0.000065	-1.302274	B	1.519536	0.006697	1.157489
B	0.898341	1.466116	-0.50408	B	0.928749	-1.47215	0.299689
B	-0.898413	1.466129	-0.504064	B	-0.911612	-1.470148	0.387636
B	-1.463192	0.000031	-1.302365	B	-1.414927	0.00988	1.297551
B	0.898433	-1.466045	-0.504215	B	0.930916	1.47407	0.278766
B	1.449242	-0.000013	0.435289	B	1.449736	-0.005988	-0.635587
B	-0.000036	0.912479	0.955933	B	-0.059733	-0.910679	-1.100788
B	-1.449297	-0.000103	0.435209	B	-1.515881	-0.002786	-0.494043
B	-0.898326	-1.466143	-0.504288	B	-0.90944	1.476066	0.366723
B	-0.000045	-0.912617	0.955831	B	-0.058395	0.894237	-1.113603
I	3.287359	0.000197	-2.553362	I	3.29685	0.014739	2.473397
I	2.054027	3.344811	-0.560094	I	2.061832	-3.353075	0.392155
I	-2.054144	3.34476	-0.560183	I	-2.034728	-3.348679	0.587345
I	-3.287307	0.000231	-2.55348	I	-3.059986	0.021548	2.775129
I	2.054312	-3.344603	-0.560544	I	2.066753	3.35446	0.344526
I	3.307373	0.000026	1.624715	I	3.277815	-0.015961	-1.850227
I	-0.000104	2.090134	2.825433	I	-0.14926	-2.098392	-2.94771
I	-3.307475	-0.000265	1.624564	I	-3.451473	-0.008709	-1.528859
I	-2.054016	-3.34484	-0.56045	I	-2.029806	3.358888	0.539722
I	-0.00004	-2.09054	2.825166	I	-0.146178	2.055739	-2.977205
O	0.000445	0.759275	-3.370355	O	0.959653	0.078305	6.527746
O	-0.000267	-0.758614	-3.37066	O	0.090876	0.037084	5.679257

Table S47: Optimized geometry in Å for the species in Figure 5 of the main text.

XII			
Atom	x	y	z
B	0.006064	0.713165	-1.713651
B	0.000936	-1.010136	-1.914336
B	1.48405	-0.037401	-1.346115
B	0.919755	1.45984	-0.470937
B	-0.915428	1.456594	-0.482448
B	-1.476166	-0.047794	-1.35761
B	0.90157	-1.453342	-0.417174
B	1.471777	0.025972	0.450817
B	-0.00124	0.949265	0.986696
B	-1.471944	0.028399	0.447159
B	-0.911807	-1.456086	-0.41161
B	-0.003743	-0.856271	1.017587
I	3.204675	-0.020325	-2.707007
I	2.02453	3.341305	-0.716748
I	-2.01661	3.338918	-0.737699
I	-3.19099	-0.022056	-2.723782
I	2.04302	-3.341808	-0.482085
I	3.362491	0.06471	1.569297
I	-0.00438	2.190213	2.799096
I	-3.367062	0.083	1.556764
I	-2.059925	-3.33506	-0.450882
I	-0.001369	-1.973114	2.91324
O	-0.005892	-1.691533	-3.121554
H	0.325893	-2.595286	-3.0397

Table S48: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition states in Figure 5 of the main text.

TS5				TS6			
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
-863.996	653.2471	523.4569	32.6041	-787.8215	482.6286	434.7265	1.6543
46.8076	0.661	549.9769	7.8967	49.426	0	445.0049	5.3665
49.0511	1.7524	553.8729	0.7534	49.8671	0.0019	498.4952	20.3442
52.2169	0.1284	559.0441	4.8469	52.025	0.1345	510.1031	3.5852
54.2536	1.2811	566.4216	9.9304	55.5178	0.0319	518.0034	0.0002
55.1268	0.0402	569.1555	4.4441	56.7398	0	520.9522	33.4253
57.0948	0.1592	615.1034	43.2735	58.9586	0.0409	552.8918	17.7824
58.7396	0.0139	627.2422	1.5235	59.9145	0.0147	571.2901	0
65.0391	0.0153	635.616	0.5599	65.738	0.0582	580.4918	0.7468
66.6254	0.0855	650.544	44.8482	67.3768	0	607.844	0.0003
67.421	0.0394	693.4405	0.7001	67.9416	0.0197	609.0744	14.5876
68.3803	0.2037	702.2833	0.9391	71.9031	0.0191	619.8246	0.2143
68.6203	0.0222	708.0841	1.9173	72.2622	0.0338	642.4504	9.5338
70.5612	0.0367	710.3134	4.5902	72.4615	0	661.9932	45.1823
72.3557	5.2127	714.461	5.1426	72.5036	0.0008	678.908	3.9466
75.2075	3.6077	717.7436	0.8875	80.8934	0.8428	683.2728	15.4396
79.2554	0.1883	752.3631	0.7268	81.3145	0.0314	713.9522	0
83.6298	0.127	754.0599	3.5302	85.0226	0.1921	724.7418	86.3009
88.1992	21.1685	769.6249	4.7897	109.5518	3.0871	784.7105	2.5209
136.4301	0.691	773.6877	1.9372	131.0695	0	792.8528	1.9361
137.1116	0.0485	819.094	0.0544	133.3591	0.1903	808.3766	29.7203
137.8262	0.0077	829.6123	12.7835	134.8756	0.6493	809.3036	21.0968
138.8823	0.0004	855.0176	1.8096	136.3211	0.4568	845.1672	0
141.5825	0.0986	882.3638	11.8512	137.0185	0.1113	851.3947	51.2951
143.45	0.0214	885.7639	55.737	139.5976	0.3196	857.1596	0.0019
145.2602	0.0254	891.6771	9.5154	144.9058	0.0147	873.1271	92.0545
157.0929	3.5349	898.7318	83.7723	153.0417	1.4361	885.3818	150.858
187.4046	11.4959	901.8995	14.7137	206.6345	0	892.8734	74.5454
202.7216	1.8526	908.0326	141.749	214.3405	7.9962	894.6312	306.6169
247.4138	6.8482	927.2601	146.7518	248.7894	3.1027	949.1165	4.7481
305.6724	0.9938	1033.9769	146.7873	289.9837	0.8282	1449.3496	3.9391
320.7581	7.6239	1090.2501	77.6189	359.2591	4.9222	1489.1958	56.7258
360.3857	18.5147	1127.3068	15.0847	362.4877	12.9028	3126.8032	787.8775
374.5251	0.9364	1179.0669	16.4872	371.4636	0		
387.5668	34.2177	1190.4807	15.7092	380.8269	3.7827		
408.6877	13.7387	1437.5459	91.602	391.0138	50.884		
436.5545	44.202	1559.888	38.9933	402.2792	25.6584		
483.3492	24.8215	3617.6254	132.9853	409.788	42.574		
497.54	15.3035	3746.5409	72.2704	412.9374	0		

Table S49: Harmonic frequencies (cm^{-1}) and intensities (km mol^{-1}) for the transition states in Figure 5 of the main text.

TS7				TS8			
Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
-609.8345	13.7759	557.1723	8.9988	-5.699	0.0082	530.4992	1.7423
45.3102	0.0044	570.012	1.0812	11.7918	0.0279	534.8973	0.0102
46.0845	2.7521	615.8693	0.0874	13.188	0.0057	586.8644	17.3951
50.4598	6.9182	630.8107	2.5343	16.1504	0.0146	616.3515	1.4201
51.1452	2.5033	637.8131	11.1625	30.5347	0.0264	625.5906	1.991
53.2136	0.2404	650.8586	8.7844	44.8597	0	631.524	0.0002
53.6263	0.0223	681.8829	0.063	46.0112	0.0176	681.3529	0.0476
57.9625	0.0699	682.7411	0.1485	47.2698	0.0044	684.0284	0.6328
59.8554	0.0112	693.3422	0.1814	53.8925	0	686.2251	2.1296
61.918	0.0487	716.2381	0.931	55.19	0.0006	688.5616	0.0015
63.3096	0.5842	725.6855	3.0772	55.4906	0	703.0519	49.0542
66.5824	0.4062	738.7939	0.1948	55.7587	0.0041	726.6483	22.0652
68.6617	1.0782	750.7921	0.057	61.1327	0.0747	748.6202	8.903
69.7844	0.3269	769.1991	0.0032	63.9242	0	760.4724	11.2765
70.0542	14.8657	793.15	0.2652	65.4475	0.0022	784.6845	0.0004
71.5035	6.9814	826.902	6.2129	67.4137	0.0036	809.7485	27.1955
73.453	4.3495	846.5406	3.9196	67.5771	0	821.951	0.0384
76.4118	5.8104	855.4103	12.6074	69.2783	0.0008	851.4042	39.6745
135.6984	1.0581	892.0581	0.7884	70.4522	0.0149	854.0699	9.6024
137.2203	0.4029	894.896	0.3507	77.2543	0.1726	872.962	139.8716
137.2713	0.0008	899.0574	0.6649	78.2072	0.3265	876.9858	52.0771
137.8832	0.1276	910.3827	12.7525	81.0927	0.1561	887.7986	70.4119
138.4097	0.0415	928.6897	3.0603	134.0797	0.2627	909.0446	138.4558
140.5124	0.0331	937.8228	5.4445	136.9111	0.0041	914.5126	0.1514
141.9614	0.0798	942.2985	32.5773	137.7618	0.0112	951.8016	43.1524
148.0557	0.134	1062.7947	0.0964	138.7705	0	1066.6996	1.1644
182.9824	0.7743	1126.0623	34.9276	141.7635	0.0424	1640.4573	1.4381
257.7764	1.3398			142.8476	0.0177		
266.8212	0.0025			144.6284	0.0166		
328.4957	0.282			304.955	6.1951		
354.7375	16.9174			307.3537	17.7837		
372.3075	0.0012			308.0154	7.9372		
416.698	4.2166			333.0643	0.3531		
417.0229	0.3537			339.9726	0		
477.3447	0.1919			359.6965	18.5374		
502.693	1.3318			475.8189	136.8647		
520.7558	0.0569			521.5551	0.4023		
532.9846	3.5486			524.773	4.745		
553.3817	0.0004			529.3309	6.3915		

Table S50: Calculated Gibbs energy (G), Gibbs energy within the pathway (G pathway), and relative Gibbs energy for the species shown in Figure 5 of the main text at 298.15 K.

Species	G (E_h)	G pathway (E_h)	Rel. G (eV)
VII	-565.799587	-565.799587	0
TS5	-565.804352	-565.804352	-0.13
VIII	-564.695102	-	-
H_2	-1.179849	-	-
VIII + H_2	-565.874951	-565.874951	-2.05
TS6	-564.531862		
TS6 + H_2	-565.711711	-565.711711	2.39
IX	-563.360204	-	-
IX + 2 H_2	-565.719902	-565.719902	2.17
TS7	-563.30867		-
TS7 + 2 H_2	-565.668368	-565.668368	3.57
X	-563.331025		
X + 2 H_2	-565.690723	-565.690723	2.96
TS8	-563.234808	-	-
TS8 + 2 H_2	-565.594506	-565.594506	5.58
XI	-412.902781	-	-
O_2	-150.343819	-	-
XI + 2 H_2 + O_2	-565.606298	-565.606298	5.26

Table S51: Calculated Gibbs energy (G), Gibbs energy within the pathway (G pathway), and relative Gibbs energy for the species shown in Figure 5 of the main text at 298.15 K.

Species	G (E_h)	G pathway (E_h)	Rel. G (eV)
VII	-565.799587	-565.799587	0
TS5	-565.804352	-565.804352	-0.13
VIII	-564.695102	-	-
H_2	-1.179849	-	-
VIII + H_2	-565.874951	-565.874951	-2.05
XII	-488.809256	-	-
OH	-75.747516	-	-
XII + H_2 + OH	-565.736621	-565.736621	1.71
XI	-412.902781	-	-
XI + H_2 + 2 OH	-565.577662	-565.577662	6.04

SV   Multiwfn output for ELF attractors and basins

SV.1   Output for $[B_{12}Br_{10}(H_2O)_2]^{-\bullet}$

HETATM 1 C ATT A 1 -2.302 -3.096 -1.532 0.88019514E+000 1.00 C

HETATM 2 C ATT A 2 -2.683 -2.842 -1.469 0.87881901E+000 1.00 C

HETATM 3 C ATT A 3 -3.350 -2.429 -0.389 0.88275499E+000 1.00 C

HETATM 4 C ATT A 4 -2.778 -3.032 0.627 0.87697914E+000 1.00 C

HETATM 5 C ATT A 5 -1.826 -3.699 0.246 0.88296086E+000 1.00 C

HETATM 6 C ATT A 1 -2.207 -3.191 -1.500 0.88046171E+000 1.00 C

HETATM 7 C ATT A 1 -2.143 -3.254 -1.469 0.88045243E+000 1.00 C

HETATM 8 C ATT A 6 -1.191 -1.953 -3.183 0.99823654E+000 1.00 C

HETATM 9 C ATT A 7 0.048 -1.572 -3.405 0.93150665E+000 1.00 C

HETATM 10 C ATT A 8 -0.746 -2.937 2.500 0.88285244E+000 1.00 C

HETATM 11 C ATT A 9 0.206 -2.683 -2.675 0.99790831E+000 1.00 C

HETATM 12 C ATT A 8 -0.651 -2.969 2.468 0.88289494E+000 1.00 C

HETATM 13 C ATT A 8 -0.556 -3.000 2.468 0.88292898E+000 1.00 C

HETATM 14 C ATT A 10 1.032 -3.635 -1.564 0.87909446E+000 1.00 C

HETATM 15 C ATT A 8 -0.365 -3.032 2.437 0.88298420E+000 1.00 C

HETATM 16 C ATT A 10 1.095 -3.604 -1.596 0.87924614E+000 1.00 C

HETATM 17 C ATT A 11 -0.048 -3.032 2.468 0.88295922E+000 1.00 C

HETATM 18 C ATT A 12 0.873 -4.048 0.182 0.88472680E+000 1.00 C

HETATM 19 C ATT A 11 0.111 -3.000 2.500 0.88291125E+000 1.00 C

HETATM 20 C ATT A 13 1.921 -3.350 -1.564 0.87394048E+000 1.00 C

HETATM 21 C ATT A 14 2.588 -3.254 -0.611 0.88546687E+000 1.00 C

HETATM 22 C ATT A 15 2.016 -3.699 0.405 0.87160349E+000 1.00 C

HETATM 23 C ATT A 16 2.810 -1.254 -3.024 0.88209152E+000 1.00 C

HETATM 24 C ATT A 8 -0.810 -2.905 2.500 0.88282606E+000 1.00 C

HETATM 25 C ATT A 11 0.206 -2.969 2.532 0.88289591E+000 1.00 C

HETATM 26 C ATT A 17 3.381 -1.540 1.516 0.88285791E+000 1.00 C

HETATM 27 C ATT A 2 -2.873 -2.746 -1.373 0.87820267E+000 1.00 C

HETATM 28 C ATT A 8 -0.873 -2.873 2.532 0.88282907E+000 1.00 C

HETATM 29 C ATT A 17 3.667 -1.286 1.071 0.88266361E+000 1.00 C

HETATM 30 C ATT A 17 3.254 -1.572 1.706 0.88281329E+000 1.00 C

HETATM 31 C ATT A 17 3.762 -1.127 0.944 0.88257418E+000 1.00 C

HETATM 32 C ATT A 18 1.445 -3.540 -0.294 0.78844440E+000 1.00 C

HETATM 33 C ATT A 18 1.476 -3.477 -0.262 0.78834599E+000 1.00 C

HETATM 34 C ATT A 18 1.349 -3.508 -0.294 0.78842928E+000 1.00 C

HETATM 35 C ATT A 18 1.413 -3.477 -0.262 0.78843322E+000 1.00 C

HETATM 36 C ATT A 18 1.540 -3.445 -0.262 0.78833951E+000 1.00 C

HETATM 37 C ATT A 18 1.603 -3.445 -0.294 0.78835667E+000 1.00 C

HETATM 38 C ATT A 17 3.794 -1.064 0.913 0.88254586E+000 1.00 C

HETATM 39 C ATT A 18 1.349 -3.413 -0.262 0.78828299E+000 1.00 C

HETATM 40 C ATT A 18 1.445 -3.381 -0.230 0.78647829E+000 1.00 C

HETATM 41 C ATT A 18 1.254 -3.413 -0.326 0.78826515E+000 1.00 C

HETATM 42 C ATT A 11 0.302 -2.937 2.564 0.88288251E+000 1.00 C

HETATM 43 C ATT A 18 1.572 -3.381 -0.262 0.78804645E+000 1.00 C

HETATM 44 C ATT A 19 -2.270 -3.127 -0.262 0.78828560E+000 1.00 C

HETATM 45 C ATT A 18 1.349 -3.350 -0.262 0.78808240E+000 1.00 C

HETATM 46 C ATT A 18 1.540 -3.318 -0.262 0.78792744E+000 1.00 C

HETATM 47 C ATT A 19 -2.270 -3.159 -0.357 0.78805609E+000 1.00 C

HETATM 48 C ATT A 19 -2.302 -3.096 -0.199 0.78711795E+000 1.00 C

HETATM 49 C ATT A 19 -2.207 -3.064 -0.199 0.78851339E+000 1.00 C

HETATM 50 C ATT A 19 -2.429 -3.096 -0.262 0.78761924E+000 1.00 C

HETATM 51 C ATT A 19 -2.175 -3.096 -0.262 0.78854720E+000 1.00 C

HETATM 52 C ATT A 18 1.381 -3.286 -0.262 0.78806337E+000 1.00 C

HETATM 53 C ATT A 19 -2.492 -3.064 -0.294 0.78739833E+000 1.00 C

HETATM 54 C ATT A 18 1.445 -3.254 -0.262 0.78785302E+000 1.00 C

HETATM 55 C ATT A 18 1.572 -3.254 -0.294 0.78804644E+000 1.00 C

HETATM 56 C ATT A 19 -2.429 -3.000 -0.167 0.78800287E+000 1.00 C

HETATM 57 C ATT A 19 -2.365 -3.032 -0.167 0.78826571E+000 1.00 C

HETATM 58 C ATT A 19 -2.524 -3.000 -0.262 0.78770524E+000 1.00 C

HETATM 59 C ATT A 19 -2.080 -3.000 -0.262 0.78831007E+000 1.00 C

HETATM 60 C ATT A 18 1.318 -3.223 -0.326 0.78818851E+000 1.00 C

HETATM 61 C ATT A 18 1.381 -3.223 -0.294 0.78814074E+000 1.00 C

HETATM 62 C ATT A 19 -2.524 -2.937 -0.230 0.78820464E+000 1.00 C

HETATM 63 C ATT A 19 -2.302 -3.000 -0.135 0.78840207E+000 1.00 C

HETATM 64 C ATT A 19 -2.111 -2.969 -0.199 0.78820612E+000 1.00 C

HETATM 65 C ATT A 19 -2.238 -2.969 -0.135 0.78823132E+000 1.00 C

HETATM 66 C ATT A 19 -2.175 -3.000 -0.167 0.78830708E+000 1.00 C

HETATM 67 C ATT A 17 3.826 -0.968 0.881 0.88247021E+000 1.00 C

HETATM 68 C ATT A 19 -2.461 -2.937 -0.167 0.78839056E+000 1.00 C

HETATM 69 C ATT A 19 -2.397 -2.937 -0.135 0.78839547E+000 1.00 C

HETATM 70 C ATT A 18 1.445 -3.159 -0.326 0.78728422E+000 1.00 C

HETATM 71 C ATT A 19 -2.302 -2.873 -0.103 0.78754838E+000 1.00 C

HETATM 72 C ATT A 20 1.032 -2.302 -0.357 0.88348879E+000 1.00 C

HETATM 73 C ATT A 19 -2.048 -2.873 -0.262 0.78809852E+000 1.00 C

HETATM 74 C ATT A 19 -2.524 -2.810 -0.230 0.78846102E+000 1.00 C

HETATM 75 C ATT A 19 -2.556 -2.873 -0.262 0.78818250E+000 1.00 C

HETATM 76 C ATT A 19 -2.175 -2.873 -0.135 0.78798067E+000 1.00 C

HETATM 77 C ATT A 21 -1.603 -1.953 -0.294 0.88615776E+000 1.00 C

HETATM 78 C ATT A 22 -0.206 -1.572 -0.230 0.84237646E+000 1.00 C

HETATM 79 C ATT A 19 -2.397 -2.810 -0.135 0.78829952E+000 1.00 C

HETATM 80 C ATT A 19 -2.143 -2.810 -0.167 0.78808127E+000 1.00 C

HETATM 81 C ATT A 11 0.365 -2.905 2.595 0.88289625E+000 1.00 C

HETATM 82 C ATT A 19 -2.238 -2.778 -0.135 0.78806121E+000 1.00 C

HETATM 83 C ATT A 19 -2.238 -2.715 -0.167 0.78806362E+000 1.00 C

HETATM 84 C ATT A 19 -2.016 -2.842 -0.389 0.78811404E+000 1.00 C

HETATM 85 C ATT A 17 3.858 -0.905 0.849 0.88243589E+000 1.00 C

HETATM 86 C ATT A 19 -2.492 -2.746 -0.230 0.78839108E+000 1.00 C

HETATM 87 C ATT A 19 -2.365 -2.683 -0.199 0.78805672E+000 1.00 C

HETATM 88 C ATT A 19 -2.238 -2.651 -0.230 0.78821462E+000 1.00 C

HETATM 89 C ATT A 19 -2.143 -2.683 -0.262 0.78826757E+000 1.00 C

HETATM 90 C ATT A 19 -2.302 -2.588 -0.389 0.78780013E+000 1.00 C

HETATM 91 C ATT A 19 -2.365 -2.619 -0.294 0.78810287E+000 1.00 C

HETATM 92 C ATT A 23 -1.191 -2.588 2.691 0.88316287E+000 1.00 C

HETATM 93 C ATT A 17 3.889 -0.778 0.817 0.88240410E+000 1.00 C

HETATM 94 C ATT A 24 -3.889 -0.238 1.071 0.88298079E+000 1.00 C

HETATM 95 C ATT A 24 -3.921 -0.111 0.976 0.88300764E+000 1.00 C

HETATM 96 C ATT A 25 0.365 -1.318 0.500 0.85762144E+000 1.00 C

HETATM 97 C ATT A 26 0.714 -1.540 -0.294 0.99999939E+000 1.00 C

HETATM 98 C ATT A 17 3.921 -0.683 0.817 0.88237494E+000 1.00 C

HETATM 99 C ATT A 17 3.604 -1.381 1.167 0.88264048E+000 1.00 C

HETATM 100 C ATT A 27 -0.683 -1.191 0.500 0.85990424E+000 1.00 C

HETATM 101 C ATT A 28 1.159 -0.968 0.214 0.86174128E+000 1.00 C

HETATM 102 C ATT A 29 -1.064 -1.318 -0.294 0.99999958E+000 1.00 C

HETATM 103 C ATT A 30 2.143 -0.302 1.008 0.89505552E+000 1.00 C

HETATM 104 C ATT A 31 3.953 -0.270 0.817 0.88262537E+000 1.00 C

HETATM 105 C ATT A 11 0.460 -2.842 2.627 0.88291060E+000 1.00 C

HETATM 106 C ATT A 32 -1.381 -0.619 0.214 0.85957773E+000 1.00 C

HETATM 107 C ATT A 24 -3.953 0.016 0.913 0.88292319E+000 1.00 C

HETATM 108 C ATT A 33 1.222 -0.937 -0.738 0.84318964E+000 1.00 C

HETATM 109 C ATT A 34 1.603 -0.206 -0.326 0.85198673E+000 1.00 C

HETATM 110 C ATT A 35 -2.143 0.302 1.008 0.89505955E+000 1.00 C

HETATM 111 C ATT A 36 -2.873 -0.556 -3.120 0.87986552E+000 1.00 C

HETATM 112 C ATT A 24 -3.953 0.079 0.881 0.88286976E+000 1.00 C

HETATM 113 C ATT A 37 -1.603 0.206 -0.326 0.85198977E+000 1.00 C

HETATM 114 C ATT A 24 -3.953 0.175 0.849 0.88275743E+000 1.00 C

HETATM 115 C ATT A 11 0.587 -2.746 2.722 0.88287424E+000 1.00 C

HETATM 116 C ATT A 17 3.191 -1.540 1.833 0.88303270E+000 1.00 C

HETATM 117 C ATT A 38 0.714 -0.556 1.008 0.84872835E+000 1.00 C

HETATM 118 C ATT A 31 3.953 -0.079 0.881 0.88286883E+000 1.00 C

HETATM 119 C ATT A 39 -0.841 -0.365 0.976 0.84742053E+000 1.00 C

HETATM 120 C ATT A 40 0.016 -0.016 1.294 0.86463699E+000 1.00 C

HETATM 121 C ATT A 41 0.841 0.365 0.976 0.84744134E+000 1.00 C

HETATM 122 C ATT A 42 1.381 0.619 0.214 0.85959378E+000 1.00 C

HETATM 123 C ATT A 24 -3.953 0.270 0.817 0.88262600E+000 1.00 C

HETATM 124 C ATT A 43 -1.159 0.968 0.214 0.86173359E+000 1.00 C

HETATM 125 C ATT A 44 -0.714 0.556 1.008 0.84873532E+000 1.00 C

HETATM 126 C ATT A 45 -1.222 0.937 -0.738 0.84321598E+000 1.00 C

HETATM 127 C ATT A 46 -0.365 1.318 0.500 0.85764273E+000 1.00 C

HETATM 128 C ATT A 47 0.683 1.191 0.500 0.85988309E+000 1.00 C

HETATM 129 C ATT A 31 3.953 -0.016 0.913 0.88292305E+000 1.00 C

HETATM 130 C ATT A 31 3.921 0.111 0.976 0.88300394E+000 1.00 C

HETATM 131 C ATT A 48 -3.921 0.683 0.817 0.88237759E+000 1.00 C

HETATM 132 C ATT A 48 -3.889 0.778 0.817 0.88240472E+000 1.00 C

HETATM 133 C ATT A 48 -3.858 0.905 0.849 0.88243407E+000 1.00 C

HETATM 134 C ATT A 31 3.889 0.238 1.071 0.88297624E+000 1.00 C

HETATM 135 C ATT A 48 -3.826 0.968 0.881 0.88247628E+000 1.00 C

HETATM 136 C ATT A 49 0.206 1.572 -0.230 0.84235481E+000 1.00 C

HETATM 137 C ATT A 50 1.603 1.953 -0.294 0.88615979E+000 1.00 C

HETATM 138 C ATT A 51 3.350 2.429 -0.389 0.88275463E+000 1.00 C

HETATM 139 C ATT A 48 -3.794 1.064 0.913 0.88254529E+000 1.00 C

HETATM 140 C ATT A 52 1.064 1.318 -0.294 0.99999958E+000 1.00 C

HETATM 141 C ATT A 48 -3.762 1.127 0.944 0.88257355E+000 1.00 C

HETATM 142 C ATT A 53 -0.714 1.540 -0.294 0.99999939E+000 1.00 C

HETATM 143 C ATT A 48 -3.699 1.222 1.008 0.88262090E+000 1.00 C

HETATM 144 C ATT A 11 0.683 -2.619 2.786 0.88282886E+000 1.00 C

HETATM 145 C ATT A 48 -3.667 1.286 1.071 0.88266655E+000 1.00 C

HETATM 146 C ATT A 54 -1.032 2.302 -0.357 0.88350085E+000 1.00 C

HETATM 147 C ATT A 17 3.127 -1.508 1.960 0.88298928E+000 1.00 C

HETATM 148 C ATT A 48 -3.604 1.381 1.167 0.88263918E+000 1.00 C

HETATM 149 C ATT A 55 -2.588 3.254 -0.611 0.88546332E+000 1.00 C

HETATM 150 C ATT A 11 0.746 -2.524 2.849 0.88270869E+000 1.00 C

HETATM 151 C ATT A 56 -3.477 -0.714 -2.453 0.87530365E+000 1.00 C

HETATM 152 C ATT A 56 -3.540 -0.683 -2.358 0.87516283E+000 1.00 C

HETATM 153 C ATT A 57 2.238 2.651 -0.230 0.78821726E+000 1.00 C

HETATM 154 C ATT A 57 2.302 2.588 -0.389 0.78779419E+000 1.00 C

HETATM 155 C ATT A 57 2.365 2.619 -0.294 0.78810320E+000 1.00 C

HETATM 156 C ATT A 57 2.365 2.683 -0.199 0.78805559E+000 1.00 C

HETATM 157 C ATT A 57 2.143 2.651 -0.326 0.78847564E+000 1.00 C

HETATM 158 C ATT A 58 -3.953 0.016 -1.786 0.88068776E+000 1.00 C

HETATM 159 C ATT A 57 2.492 2.746 -0.230 0.78839085E+000 1.00 C

HETATM 160 C ATT A 57 2.207 2.619 -0.326 0.78832058E+000 1.00 C

HETATM 161 C ATT A 57 2.080 2.746 -0.262 0.78815282E+000 1.00 C

HETATM 162 C ATT A 57 2.143 2.810 -0.167 0.78807516E+000 1.00 C

HETATM 163 C ATT A 57 2.238 2.715 -0.167 0.78806926E+000 1.00 C

HETATM 164 C ATT A 57 2.302 2.873 -0.103 0.78757882E+000 1.00 C

HETATM 165 C ATT A 57 2.397 2.810 -0.135 0.78830042E+000 1.00 C

HETATM 166 C ATT A 23 -1.254 -2.492 2.754 0.88325199E+000 1.00 C

HETATM 167 C ATT A 17 3.064 -1.476 2.056 0.88288348E+000 1.00 C

HETATM 168 C ATT A 59 1.826 3.699 0.246 0.88295724E+000 1.00 C

HETATM 169 C ATT A 57 2.238 2.778 -0.135 0.78805697E+000 1.00 C

HETATM 170 C ATT A 57 2.016 2.842 -0.389 0.78811950E+000 1.00 C

HETATM 171 C ATT A 57 2.524 2.810 -0.230 0.78845739E+000 1.00 C

HETATM 172 C ATT A 60 3.953 -0.206 -1.723 0.88075561E+000 1.00 C

HETATM 173 C ATT A 61 -0.873 4.048 0.182 0.88472738E+000 1.00 C

HETATM 174 C ATT A 57 2.175 2.873 -0.135 0.78800207E+000 1.00 C

HETATM 175 C ATT A 57 2.048 2.905 -0.262 0.78809826E+000 1.00 C

HETATM 176 C ATT A 57 2.556 2.873 -0.262 0.78816921E+000 1.00 C

HETATM 177 C ATT A 57 2.111 2.969 -0.199 0.78822150E+000 1.00 C

HETATM 178 C ATT A 57 2.397 2.937 -0.135 0.78839121E+000 1.00 C

HETATM 179 C ATT A 57 2.461 2.937 -0.167 0.78839020E+000 1.00 C

HETATM 180 C ATT A 57 2.524 2.937 -0.230 0.78820653E+000 1.00 C

HETATM 181 C ATT A 62 -2.016 3.699 0.405 0.87161382E+000 1.00 C

HETATM 182 C ATT A 57 2.175 3.000 -0.167 0.78832589E+000 1.00 C

HETATM 183 C ATT A 57 2.302 3.000 -0.135 0.78841257E+000 1.00 C

HETATM 184 C ATT A 57 2.429 3.000 -0.167 0.78800747E+000 1.00 C

HETATM 185 C ATT A 63 -1.445 3.254 -0.262 0.78787144E+000 1.00 C

HETATM 186 C ATT A 63 -1.445 3.159 -0.326 0.78732570E+000 1.00 C

HETATM 187 C ATT A 63 -1.381 3.223 -0.294 0.78813734E+000 1.00 C

HETATM 188 C ATT A 57 2.080 3.000 -0.262 0.78831035E+000 1.00 C

HETATM 189 C ATT A 63 -1.572 3.254 -0.294 0.78804825E+000 1.00 C

HETATM 190 C ATT A 57 2.365 3.032 -0.167 0.78825751E+000 1.00 C

HETATM 191 C ATT A 63 -1.445 3.381 -0.230 0.78652346E+000 1.00 C

HETATM 192 C ATT A 57 2.207 3.064 -0.199 0.78852100E+000 1.00 C

HETATM 193 C ATT A 57 2.524 3.000 -0.262 0.78769804E+000 1.00 C

HETATM 194 C ATT A 63 -1.540 3.318 -0.262 0.78791191E+000 1.00 C

HETATM 195 C ATT A 63 -1.381 3.286 -0.262 0.78806700E+000 1.00 C

HETATM 196 C ATT A 63 -1.318 3.223 -0.326 0.78818019E+000 1.00 C

HETATM 197 C ATT A 63 -1.349 3.350 -0.262 0.78807304E+000 1.00 C

HETATM 198 C ATT A 57 2.175 3.096 -0.262 0.78854255E+000 1.00 C

HETATM 199 C ATT A 57 2.302 3.096 -0.199 0.78715061E+000 1.00 C

HETATM 200 C ATT A 57 2.270 3.127 -0.262 0.78828075E+000 1.00 C

HETATM 201 C ATT A 57 2.270 3.159 -0.357 0.78805541E+000 1.00 C

HETATM 202 C ATT A 57 2.429 3.096 -0.262 0.78761745E+000 1.00 C

HETATM 203 C ATT A 57 2.492 3.064 -0.294 0.78739626E+000 1.00 C

HETATM 204 C ATT A 64 2.778 3.032 0.627 0.87698311E+000 1.00 C

HETATM 205 C ATT A 63 -1.572 3.381 -0.262 0.78805998E+000 1.00 C

HETATM 206 C ATT A 63 -1.349 3.413 -0.262 0.78828419E+000 1.00 C

HETATM 207 C ATT A 63 -1.254 3.413 -0.326 0.78826320E+000 1.00 C

HETATM 208 C ATT A 63 -1.603 3.445 -0.294 0.78835595E+000 1.00 C

HETATM 209 C ATT A 63 -1.540 3.445 -0.262 0.78834231E+000 1.00 C

HETATM 210 C ATT A 63 -1.476 3.477 -0.262 0.78834051E+000 1.00 C

HETATM 211 C ATT A 63 -1.413 3.477 -0.262 0.78843413E+000 1.00 C

HETATM 212 C ATT A 63 -1.349 3.508 -0.294 0.78843481E+000 1.00 C

HETATM 213 C ATT A 17 3.032 -1.445 2.119 0.88277502E+000 1.00 C

HETATM 214 C ATT A 63 -1.445 3.540 -0.294 0.78844429E+000 1.00 C

HETATM 215 C ATT A 23 -1.286 -2.429 2.786 0.88330416E+000 1.00 C

HETATM 216 C ATT A 11 0.778 -2.461 2.913 0.88261960E+000 1.00 C

HETATM 217 C ATT A 65 -3.572 -0.619 1.706 0.88263162E+000 1.00 C

HETATM 218 C ATT A 23 -1.318 -2.365 2.818 0.88328530E+000 1.00 C

HETATM 219 C ATT A 65 -3.540 -0.619 1.802 0.88259254E+000 1.00 C

HETATM 220 C ATT A 65 -3.445 -0.619 1.929 0.88262603E+000 1.00 C

HETATM 221 C ATT A 23 -1.349 -2.238 2.881 0.88323169E+000 1.00 C

HETATM 222 C ATT A 17 3.000 -1.381 2.214 0.88261123E+000 1.00 C

HETATM 223 C ATT A 65 -3.350 -0.587 2.087 0.88253671E+000 1.00 C

HETATM 224 C ATT A 11 0.810 -2.365 2.976 0.88246486E+000 1.00 C

HETATM 225 C ATT A 66 2.873 0.556 -3.120 0.87986945E+000 1.00 C

HETATM 226 C ATT A 60 3.953 -0.111 -1.754 0.88083018E+000 1.00 C

HETATM 227 C ATT A 67 3.477 0.714 -2.453 0.87528194E+000 1.00 C

HETATM 228 C ATT A 67 3.540 0.683 -2.358 0.87514486E+000 1.00 C

HETATM 229 C ATT A 65 -3.318 -0.556 2.151 0.88245381E+000 1.00 C

HETATM 230 C ATT A 68 0.016 -0.016 -1.945 0.87088907E+000 1.00 C

HETATM 231 C ATT A 58 -3.953 0.111 -1.754 0.88082407E+000 1.00 C

HETATM 232 C ATT A 69 -0.048 1.572 -3.405 0.93149544E+000 1.00 C

HETATM 233 C ATT A 17 3.445 -1.508 1.421 0.88277719E+000 1.00 C

HETATM 234 C ATT A 70 -2.810 1.254 -3.024 0.88209133E+000 1.00 C

HETATM 235 C ATT A 58 -3.953 0.175 -1.723 0.88075863E+000 1.00 C

HETATM 236 C ATT A 11 0.841 -2.207 3.072 0.88219535E+000 1.00 C

HETATM 237 C ATT A 65 -3.604 -0.619 1.643 0.88260195E+000 1.00 C

HETATM 238 C ATT A 65 -3.254 -0.524 2.214 0.88236729E+000 1.00 C

HETATM 239 C ATT A 71 -1.286 -1.762 3.230 0.88227946E+000 1.00 C

HETATM 240 C ATT A 72 -0.841 -1.318 3.548 0.88255700E+000 1.00 C

HETATM 241 C ATT A 73 0.143 -1.286 3.643 0.88349428E+000 1.00 C

HETATM 242 C ATT A 73 0.524 -1.508 3.516 0.88343979E+000 1.00 C

HETATM 243 C ATT A 11 0.778 -1.857 3.294 0.88239918E+000 1.00 C

HETATM 244 C ATT A 11 0.810 -1.984 3.230 0.88225396E+000 1.00 C

HETATM 245 C ATT A 11 0.841 -2.111 3.135 0.88213198E+000 1.00 C

HETATM 246 C ATT A 71 -1.318 -1.857 3.167 0.88242069E+000 1.00 C

HETATM 247 C ATT A 71 -1.254 -1.699 3.262 0.88222561E+000 1.00 C

HETATM 248 C ATT A 72 -1.032 -1.445 3.453 0.88233548E+000 1.00 C

HETATM 249 C ATT A 72 -0.651 -1.254 3.611 0.88275786E+000 1.00 C

HETATM 250 C ATT A 73 -0.016 -1.254 3.675 0.88327235E+000 1.00 C

HETATM 251 C ATT A 73 0.460 -1.445 3.548 0.88353169E+000 1.00 C

HETATM 252 C ATT A 71 -1.222 -1.635 3.294 0.88218153E+000 1.00 C

HETATM 253 C ATT A 74 -3.572 1.318 -2.167 0.87441172E+000 1.00 C

HETATM 254 C ATT A 73 -0.111 -1.222 3.675 0.88316773E+000 1.00 C

HETATM 255 C ATT A 75 1.191 1.953 -3.183 0.99824556E+000 1.00 C

HETATM 256 C ATT A 72 -0.746 -1.286 3.580 0.88269011E+000 1.00 C

HETATM 257 C ATT A 72 -0.587 -1.222 3.611 0.88280624E+000 1.00 C

HETATM 258 C ATT A 73 0.079 -1.254 3.643 0.88340257E+000 1.00 C

HETATM 259 C ATT A 73 0.238 -1.318 3.611 0.88353722E+000 1.00 C

HETATM 260 C ATT A 73 0.302 -1.349 3.611 0.88356705E+000 1.00 C

HETATM 261 C ATT A 17 3.477 -1.476 1.325 0.88269374E+000 1.00 C

HETATM 262 C ATT A 73 0.397 -1.413 3.580 0.88359854E+000 1.00 C

HETATM 263 C ATT A 72 -0.492 -1.222 3.643 0.88288235E+000 1.00 C

HETATM 264 C ATT A 65 -3.223 -0.492 2.278 0.88229750E+000 1.00 C

HETATM 265 C ATT A 17 3.572 -1.413 1.230 0.88268638E+000 1.00 C

HETATM 266 C ATT A 76 2.873 -1.032 2.532 0.88200310E+000 1.00 C

HETATM 267 C ATT A 76 2.842 -0.968 2.564 0.88200083E+000 1.00 C

HETATM 268 C ATT A 76 2.842 -0.905 2.595 0.88203813E+000 1.00 C

HETATM 269 C ATT A 76 2.842 -0.810 2.627 0.88205415E+000 1.00 C

HETATM 270 C ATT A 77 -3.064 -0.270 2.500 0.88204722E+000 1.00 C

HETATM 271 C ATT A 65 -3.667 -0.587 1.548 0.88261738E+000 1.00 C

HETATM 272 C ATT A 76 2.810 -0.683 2.659 0.88216937E+000 1.00 C

HETATM 273 C ATT A 77 -3.000 -0.175 2.564 0.88205146E+000 1.00 C

HETATM 274 C ATT A 76 2.810 -0.524 2.691 0.88231185E+000 1.00 C

HETATM 275 C ATT A 77 -2.969 -0.111 2.595 0.88208368E+000 1.00 C

HETATM 276 C ATT A 78 2.873 -0.206 2.691 0.88235521E+000 1.00 C

HETATM 277 C ATT A 79 3.318 0.556 2.151 0.88245399E+000 1.00 C

HETATM 278 C ATT A 78 2.937 0.016 2.627 0.88212850E+000 1.00 C

HETATM 279 C ATT A 78 3.000 0.175 2.564 0.88204808E+000 1.00 C

HETATM 280 C ATT A 78 3.064 0.270 2.500 0.88204615E+000 1.00 C

HETATM 281 C ATT A 79 3.254 0.524 2.214 0.88236724E+000 1.00 C

HETATM 282 C ATT A 79 3.350 0.587 2.087 0.88253567E+000 1.00 C

HETATM 283 C ATT A 79 3.445 0.619 1.929 0.88262580E+000 1.00 C

HETATM 284 C ATT A 79 3.667 0.587 1.548 0.88261672E+000 1.00 C

HETATM 285 C ATT A 79 3.699 0.556 1.484 0.88265226E+000 1.00 C

HETATM 286 C ATT A 79 3.794 0.460 1.294 0.88275567E+000 1.00 C

HETATM 287 C ATT A 78 2.905 -0.079 2.659 0.88223602E+000 1.00 C

HETATM 288 C ATT A 79 3.223 0.492 2.278 0.88229575E+000 1.00 C

HETATM 289 C ATT A 79 3.604 0.619 1.643 0.88260083E+000 1.00 C

HETATM 290 C ATT A 77 -2.937 -0.016 2.627 0.88212877E+000 1.00 C

HETATM 291 C ATT A 79 3.572 0.619 1.706 0.88263055E+000 1.00 C

HETATM 292 C ATT A 79 3.540 0.619 1.802 0.88259263E+000 1.00 C

HETATM 293 C ATT A 78 2.969 0.111 2.595 0.88208005E+000 1.00 C

HETATM 294 C ATT A 65 -3.699 -0.556 1.484 0.88265407E+000 1.00 C

HETATM 295 C ATT A 77 -2.905 0.079 2.659 0.88223726E+000 1.00 C

HETATM 296 C ATT A 77 -2.873 0.206 2.691 0.88235863E+000 1.00 C

HETATM 297 C ATT A 65 -3.794 -0.460 1.294 0.88275621E+000 1.00 C

HETATM 298 C ATT A 80 -0.206 2.683 -2.675 0.99790390E+000 1.00 C

HETATM 299 C ATT A 81 0.746 1.286 3.580 0.88269137E+000 1.00 C

HETATM 300 C ATT A 81 0.651 1.254 3.611 0.88275961E+000 1.00 C

HETATM 301 C ATT A 81 0.841 1.318 3.548 0.88256020E+000 1.00 C

HETATM 302 C ATT A 81 0.587 1.222 3.611 0.88280763E+000 1.00 C

HETATM 303 C ATT A 81 0.492 1.222 3.643 0.88288318E+000 1.00 C

HETATM 304 C ATT A 82 0.111 1.222 3.675 0.88316773E+000 1.00 C

HETATM 305 C ATT A 83 -1.095 3.604 -1.596 0.87925524E+000 1.00 C

HETATM 306 C ATT A 82 0.016 1.254 3.675 0.88327195E+000 1.00 C

HETATM 307 C ATT A 82 -0.079 1.254 3.643 0.88340193E+000 1.00 C

HETATM 308 C ATT A 82 -0.143 1.286 3.643 0.88349347E+000 1.00 C

HETATM 309 C ATT A 82 -0.238 1.318 3.611 0.88353664E+000 1.00 C

HETATM 310 C ATT A 82 -0.302 1.349 3.611 0.88356511E+000 1.00 C

HETATM 311 C ATT A 82 -0.397 1.413 3.580 0.88359687E+000 1.00 C

HETATM 312 C ATT A 84 -2.810 0.524 2.691 0.88231597E+000 1.00 C

HETATM 313 C ATT A 82 -0.460 1.445 3.548 0.88352955E+000 1.00 C

HETATM 314 C ATT A 85 2.302 3.096 -1.532 0.88019399E+000 1.00 C

HETATM 315 C ATT A 82 -0.524 1.508 3.516 0.88343871E+000 1.00 C

HETATM 316 C ATT A 86 2.683 2.842 -1.469 0.87882163E+000 1.00 C

HETATM 317 C ATT A 81 1.032 1.445 3.453 0.88233732E+000 1.00 C

HETATM 318 C ATT A 86 2.873 2.746 -1.373 0.87820693E+000 1.00 C

HETATM 319 C ATT A 87 1.222 1.635 3.294 0.88218309E+000 1.00 C

HETATM 320 C ATT A 84 -2.810 0.683 2.659 0.88217130E+000 1.00 C

HETATM 321 C ATT A 48 -3.000 1.381 2.214 0.88261260E+000 1.00 C

HETATM 322 C ATT A 84 -2.810 0.810 2.627 0.88205659E+000 1.00 C

HETATM 323 C ATT A 48 -3.572 1.413 1.230 0.88268869E+000 1.00 C

HETATM 324 C ATT A 48 -3.127 1.508 1.960 0.88299054E+000 1.00 C

HETATM 325 C ATT A 88 -1.921 3.350 -1.564 0.87395317E+000 1.00 C

HETATM 326 C ATT A 84 -2.873 1.032 2.532 0.88200493E+000 1.00 C

HETATM 327 C ATT A 84 -2.842 0.968 2.564 0.88200449E+000 1.00 C

HETATM 328 C ATT A 84 -2.842 0.905 2.595 0.88204104E+000 1.00 C

HETATM 329 C ATT A 48 -3.381 1.540 1.516 0.88285867E+000 1.00 C

HETATM 330 C ATT A 48 -3.191 1.540 1.833 0.88303449E+000 1.00 C

HETATM 331 C ATT A 48 -3.032 1.445 2.119 0.88277679E+000 1.00 C

HETATM 332 C ATT A 48 -3.477 1.476 1.325 0.88269795E+000 1.00 C

HETATM 333 C ATT A 48 -3.445 1.508 1.421 0.88277952E+000 1.00 C

HETATM 334 C ATT A 48 -3.254 1.572 1.706 0.88281152E+000 1.00 C

HETATM 335 C ATT A 48 -3.064 1.476 2.056 0.88288499E+000 1.00 C

HETATM 336 C ATT A 87 1.254 1.699 3.262 0.88222634E+000 1.00 C

HETATM 337 C ATT A 85 2.207 3.191 -1.500 0.88046394E+000 1.00 C

HETATM 338 C ATT A 87 1.286 1.762 3.230 0.88228137E+000 1.00 C

HETATM 339 C ATT A 87 1.318 1.857 3.167 0.88242032E+000 1.00 C

HETATM 340 C ATT A 89 -0.778 1.857 3.294 0.88239891E+000 1.00 C

HETATM 341 C ATT A 90 1.349 2.238 2.881 0.88323158E+000 1.00 C

HETATM 342 C ATT A 89 -0.810 1.984 3.230 0.88225445E+000 1.00 C

HETATM 343 C ATT A 85 2.143 3.254 -1.469 0.88045661E+000 1.00 C

HETATM 344 C ATT A 89 -0.841 2.111 3.135 0.88212986E+000 1.00 C

HETATM 345 C ATT A 89 -0.841 2.207 3.072 0.88219359E+000 1.00 C

HETATM 346 C ATT A 89 -0.810 2.365 2.976 0.88246477E+000 1.00 C

HETATM 347 C ATT A 89 -0.587 2.746 2.722 0.88287277E+000 1.00 C

HETATM 348 C ATT A 90 1.191 2.588 2.691 0.88316101E+000 1.00 C

HETATM 349 C ATT A 90 1.318 2.365 2.818 0.88328628E+000 1.00 C

HETATM 350 C ATT A 89 -0.778 2.461 2.913 0.88261936E+000 1.00 C

HETATM 351 C ATT A 89 -0.683 2.619 2.786 0.88283088E+000 1.00 C

HETATM 352 C ATT A 89 0.048 3.032 2.468 0.88295859E+000 1.00 C

HETATM 353 C ATT A 91 0.556 3.000 2.468 0.88292701E+000 1.00 C

HETATM 354 C ATT A 90 1.286 2.429 2.786 0.88330321E+000 1.00 C

HETATM 355 C ATT A 89 -0.746 2.524 2.849 0.88270955E+000 1.00 C

HETATM 356 C ATT A 89 -0.365 2.905 2.595 0.88289561E+000 1.00 C

HETATM 357 C ATT A 90 1.254 2.492 2.754 0.88325085E+000 1.00 C

HETATM 358 C ATT A 89 -0.206 2.969 2.532 0.88289645E+000 1.00 C

HETATM 359 C ATT A 91 0.365 3.032 2.437 0.88298292E+000 1.00 C

HETATM 360 C ATT A 91 0.746 2.937 2.500 0.88285004E+000 1.00 C

HETATM 361 C ATT A 83 -1.032 3.635 -1.564 0.87910481E+000 1.00 C

HETATM 362 C ATT A 89 -0.460 2.842 2.627 0.88291052E+000 1.00 C

HETATM 363 C ATT A 89 -0.111 3.000 2.500 0.88291091E+000 1.00 C

HETATM 364 C ATT A 91 0.651 2.969 2.468 0.88289276E+000 1.00 C

HETATM 365 C ATT A 91 0.873 2.873 2.532 0.88282679E+000 1.00 C

HETATM 366 C ATT A 89 -0.302 2.937 2.564 0.88288154E+000 1.00 C

HETATM 367 C ATT A 91 0.810 2.905 2.500 0.88282395E+000 1.00 C

HETATM 368 C ATT A 92 1.445 -0.206 0.595 0.99999949E+000 1.00 C

HETATM 369 C ATT A 93 -1.445 0.206 0.595 0.99999949E+000 1.00 C

HETATM 370 C ATT A 94 -0.175 -1.413 -2.485 0.89703142E+000 1.00 C

HETATM 371 C ATT A 95 0.175 1.413 -2.485 0.89703479E+000 1.00 C

HETATM 372 C ATT A 96 -0.873 -0.429 -1.564 0.85297436E+000 1.00 C

HETATM 373 C ATT A 97 0.873 0.429 -1.564 0.85297543E+000 1.00 C

HETATM 374 C ATT A 98 2.111 -0.270 -1.691 0.87611627E+000 1.00 C

HETATM 375 C ATT A 99 -2.111 0.270 -1.691 0.87613575E+000 1.00 C

HETATM 376 C ATT A 100 -0.206 -1.794 -2.961 0.99998903E+000 1.00 C

HETATM 377 C ATT A 101 0.746 -0.683 -1.532 0.84819083E+000 1.00 C

HETATM 378 C ATT A 102 0.206 1.794 -2.961 0.99998922E+000 1.00 C

HETATM 379 C ATT A 103 -0.746 0.683 -1.532 0.84819401E+000 1.00 C

HETATM 380 C ATT A 104 3.000 -0.333 -2.675 0.78840578E+000 1.00 C

HETATM 381 C ATT A 105 -3.000 0.333 -2.675 0.78838733E+000 1.00 C

HETATM 382 C ATT A 106 -0.175 -1.318 1.833 0.89638409E+000 1.00 C

HETATM 383 C ATT A 107 -0.111 -0.905 1.167 0.99999943E+000 1.00 C

HETATM 384 C ATT A 108 -1.667 -3.699 -0.865 0.87770153E+000 1.00 C

HETATM 385 C ATT A 108 -1.667 -3.731 -0.802 0.87771095E+000 1.00 C

HETATM 386 C ATT A 109 0.111 0.905 1.167 0.99999943E+000 1.00 C

HETATM 387 C ATT A 18 1.445 -3.635 -0.643 0.78733649E+000 1.00 C

HETATM 388 C ATT A 18 1.445 -3.667 -0.516 0.78607996E+000 1.00 C

HETATM 389 C ATT A 18 1.603 -3.540 -0.707 0.78743865E+000 1.00 C

HETATM 390 C ATT A 18 1.254 -3.508 -0.675 0.78853805E+000 1.00 C

HETATM 391 C ATT A 18 1.699 -3.508 -0.580 0.78786068E+000 1.00 C

HETATM 392 C ATT A 18 1.445 -3.572 -0.738 0.78714535E+000 1.00 C

HETATM 393 C ATT A 18 1.699 -3.445 -0.643 0.78808183E+000 1.00 C

HETATM 394 C ATT A 18 1.413 -3.508 -0.770 0.78836673E+000 1.00 C

HETATM 395 C ATT A 18 1.222 -3.445 -0.675 0.78846994E+000 1.00 C

HETATM 396 C ATT A 18 1.349 -3.477 -0.770 0.78856250E+000 1.00 C

HETATM 397 C ATT A 18 1.508 -3.508 -0.770 0.78820040E+000 1.00 C

HETATM 398 C ATT A 18 1.572 -3.445 -0.770 0.78823031E+000 1.00 C

HETATM 399 C ATT A 18 1.635 -3.413 -0.738 0.78841351E+000 1.00 C

HETATM 400 C ATT A 18 1.191 -3.445 -0.611 0.78837519E+000 1.00 C

HETATM 401 C ATT A 18 1.318 -3.413 -0.770 0.78852553E+000 1.00 C

HETATM 402 C ATT A 18 1.413 -3.413 -0.802 0.78855538E+000 1.00 C

HETATM 403 C ATT A 18 1.508 -3.413 -0.802 0.78854595E+000 1.00 C

HETATM 404 C ATT A 18 1.191 -3.381 -0.643 0.78804056E+000 1.00 C

HETATM 405 C ATT A 18 1.254 -3.381 -0.738 0.78735055E+000 1.00 C

HETATM 406 C ATT A 18 1.730 -3.350 -0.580 0.78855005E+000 1.00 C

HETATM 407 C ATT A 18 1.667 -3.318 -0.707 0.78847460E+000 1.00 C

HETATM 408 C ATT A 18 1.318 -3.318 -0.770 0.78830408E+000 1.00 C

HETATM 409 C ATT A 18 1.508 -3.350 -0.802 0.78853712E+000 1.00 C

HETATM 410 C ATT A 104 2.905 -0.333 -2.643 0.78854770E+000 1.00 C

HETATM 411 C ATT A 18 1.413 -3.318 -0.802 0.78841590E+000 1.00 C

HETATM 412 C ATT A 18 1.572 -3.286 -0.770 0.78838338E+000 1.00 C

HETATM 413 C ATT A 19 -2.302 -3.064 -0.611 0.78831052E+000 1.00 C

HETATM 414 C ATT A 104 3.096 -0.206 -2.643 0.78811553E+000 1.00 C

HETATM 415 C ATT A 104 3.000 -0.206 -2.643 0.78842559E+000 1.00 C

HETATM 416 C ATT A 18 1.191 -3.318 -0.611 0.78793577E+000 1.00 C

HETATM 417 C ATT A 18 1.381 -3.254 -0.770 0.78808420E+000 1.00 C

HETATM 418 C ATT A 110 0.175 1.318 1.833 0.89638696E+000 1.00 C

HETATM 419 C ATT A 18 1.699 -3.286 -0.643 0.78844443E+000 1.00 C

HETATM 420 C ATT A 19 -2.238 -3.000 -0.643 0.78858492E+000 1.00 C

HETATM 421 C ATT A 18 1.635 -3.254 -0.707 0.78837948E+000 1.00 C

HETATM 422 C ATT A 105 -3.096 0.206 -2.643 0.78809861E+000 1.00 C

HETATM 423 C ATT A 105 -3.000 0.206 -2.643 0.78847639E+000 1.00 C

HETATM 424 C ATT A 18 1.222 -3.254 -0.643 0.78810075E+000 1.00 C

HETATM 425 C ATT A 19 -2.365 -3.000 -0.643 0.78838628E+000 1.00 C

HETATM 426 C ATT A 18 1.286 -3.191 -0.675 0.78778603E+000 1.00 C

HETATM 427 C ATT A 18 1.413 -3.191 -0.738 0.78809097E+000 1.00 C

HETATM 428 C ATT A 18 1.508 -3.191 -0.738 0.78809208E+000 1.00 C

HETATM 429 C ATT A 19 -2.429 -2.937 -0.643 0.78838336E+000 1.00 C

HETATM 430 C ATT A 19 -2.175 -2.937 -0.643 0.78844573E+000 1.00 C

HETATM 431 C ATT A 19 -2.143 -3.064 -0.548 0.78835071E+000 1.00 C

HETATM 432 C ATT A 18 1.572 -3.191 -0.707 0.78815167E+000 1.00 C

HETATM 433 C ATT A 19 -2.492 -2.873 -0.611 0.78792016E+000 1.00 C

HETATM 434 C ATT A 19 -2.111 -2.873 -0.611 0.78803848E+000 1.00 C

HETATM 435 C ATT A 18 1.381 -3.127 -0.643 0.78806690E+000 1.00 C

HETATM 436 C ATT A 18 1.381 -3.096 -0.516 0.78847244E+000 1.00 C

HETATM 437 C ATT A 19 -2.334 -2.905 -0.675 0.78857823E+000 1.00 C

HETATM 438 C ATT A 18 1.635 -3.191 -0.643 0.78819770E+000 1.00 C

HETATM 439 C ATT A 19 -2.270 -2.905 -0.675 0.78851678E+000 1.00 C

HETATM 440 C ATT A 18 1.318 -3.127 -0.580 0.78838076E+000 1.00 C

HETATM 441 C ATT A 18 1.572 -3.127 -0.611 0.78805692E+000 1.00 C

HETATM 442 C ATT A 18 1.508 -3.096 -0.484 0.78828844E+000 1.00 C

HETATM 443 C ATT A 19 -2.429 -2.842 -0.643 0.78848820E+000 1.00 C

HETATM 444 C ATT A 19 -2.334 -2.842 -0.675 0.78850376E+000 1.00 C

HETATM 445 C ATT A 19 -2.270 -2.842 -0.675 0.78840581E+000 1.00 C

HETATM 446 C ATT A 19 -2.397 -2.778 -0.643 0.78844920E+000 1.00 C

HETATM 447 C ATT A 19 -2.207 -2.778 -0.643 0.78812260E+000 1.00 C

HETATM 448 C ATT A 19 -2.492 -2.778 -0.580 0.78853466E+000 1.00 C

HETATM 449 C ATT A 19 -2.334 -2.746 -0.643 0.78823438E+000 1.00 C

HETATM 450 C ATT A 19 -2.270 -2.746 -0.643 0.78809806E+000 1.00 C

HETATM 451 C ATT A 19 -2.302 -2.683 -0.611 0.78727926E+000 1.00 C

HETATM 452 C ATT A 19 -2.207 -2.683 -0.580 0.78810442E+000 1.00 C

HETATM 453 C ATT A 19 -2.397 -2.683 -0.580 0.78819069E+000 1.00 C

HETATM 454 C ATT A 111 0.333 -1.318 -1.088 0.86174809E+000 1.00 C

HETATM 455 C ATT A 112 -0.683 -1.159 -1.088 0.85405291E+000 1.00 C

HETATM 456 C ATT A 104 3.000 -0.460 -2.643 0.78846135E+000 1.00 C

HETATM 457 C ATT A 104 3.223 -0.333 -2.612 0.78705179E+000 1.00 C

HETATM 458 C ATT A 104 2.937 -0.238 -2.643 0.78852077E+000 1.00 C

HETATM 459 C ATT A 105 -2.905 0.206 -2.612 0.78849172E+000 1.00 C

HETATM 460 C ATT A 105 -2.905 0.333 -2.643 0.78854341E+000 1.00 C

HETATM 461 C ATT A 105 -3.223 0.333 -2.612 0.78705054E+000 1.00 C

HETATM 462 C ATT A 105 -3.000 0.460 -2.643 0.78845232E+000 1.00 C

HETATM 463 C ATT A 113 -1.413 -0.587 -0.738 0.84438626E+000 1.00 C

HETATM 464 C ATT A 104 3.032 -0.524 -2.612 0.78725479E+000 1.00 C

HETATM 465 C ATT A 105 -2.873 0.397 -2.612 0.78844382E+000 1.00 C

HETATM 466 C ATT A 105 -3.032 0.524 -2.612 0.78723074E+000 1.00 C

HETATM 467 C ATT A 104 3.127 -0.524 -2.580 0.78805041E+000 1.00 C

HETATM 468 C ATT A 104 2.937 -0.143 -2.580 0.78853008E+000 1.00 C

HETATM 469 C ATT A 105 -3.032 0.111 -2.580 0.78817121E+000 1.00 C

HETATM 470 C ATT A 104 3.032 -0.111 -2.580 0.78828116E+000 1.00 C

HETATM 471 C ATT A 105 -2.937 0.143 -2.580 0.78853633E+000 1.00 C

HETATM 472 C ATT A 114 1.413 0.587 -0.738 0.84437649E+000 1.00 C

HETATM 473 C ATT A 115 -0.333 1.318 -1.088 0.86175432E+000 1.00 C

HETATM 474 C ATT A 104 2.969 -0.556 -2.548 0.78851367E+000 1.00 C

HETATM 475 C ATT A 105 -2.969 0.556 -2.548 0.78851319E+000 1.00 C

HETATM 476 C ATT A 116 0.683 1.159 -1.088 0.85406959E+000 1.00 C

HETATM 477 C ATT A 104 2.905 -0.524 -2.548 0.78838037E+000 1.00 C

HETATM 478 C ATT A 104 2.810 -0.397 -2.548 0.78823549E+000 1.00 C

HETATM 479 C ATT A 104 3.191 -0.143 -2.548 0.78792533E+000 1.00 C

HETATM 480 C ATT A 105 -3.191 0.143 -2.548 0.78789183E+000 1.00 C

HETATM 481 C ATT A 105 -2.810 0.397 -2.548 0.78823100E+000 1.00 C

HETATM 482 C ATT A 105 -2.810 0.270 -2.548 0.78820203E+000 1.00 C

HETATM 483 C ATT A 105 -2.905 0.524 -2.548 0.78839087E+000 1.00 C

HETATM 484 C ATT A 104 3.032 -0.587 -2.516 0.78852803E+000 1.00 C

HETATM 485 C ATT A 104 3.127 -0.587 -2.485 0.78827901E+000 1.00 C

HETATM 486 C ATT A 104 3.286 -0.397 -2.516 0.78712864E+000 1.00 C

HETATM 487 C ATT A 104 2.778 -0.333 -2.516 0.78785700E+000 1.00 C

HETATM 488 C ATT A 104 3.318 -0.333 -2.326 0.78816619E+000 1.00 C

HETATM 489 C ATT A 104 3.286 -0.270 -2.516 0.78712019E+000 1.00 C

HETATM 490 C ATT A 104 2.778 -0.270 -2.485 0.78801113E+000 1.00 C

HETATM 491 C ATT A 105 -3.096 0.079 -2.516 0.78847892E+000 1.00 C

HETATM 492 C ATT A 105 -3.000 0.079 -2.516 0.78849575E+000 1.00 C

HETATM 493 C ATT A 104 2.810 -0.206 -2.516 0.78795097E+000 1.00 C

HETATM 494 C ATT A 104 3.000 -0.079 -2.516 0.78844697E+000 1.00 C

HETATM 495 C ATT A 104 3.096 -0.079 -2.516 0.78850345E+000 1.00 C

HETATM 496 C ATT A 105 -3.286 0.270 -2.516 0.78712372E+000 1.00 C

HETATM 497 C ATT A 105 -2.778 0.333 -2.516 0.78778028E+000 1.00 C

HETATM 498 C ATT A 105 -3.318 0.333 -2.326 0.78819449E+000 1.00 C

HETATM 499 C ATT A 105 -3.286 0.397 -2.516 0.78711693E+000 1.00 C

HETATM 500 C ATT A 105 -3.127 0.587 -2.485 0.78831027E+000 1.00 C

HETATM 501 C ATT A 105 -3.032 0.587 -2.516 0.78853534E+000 1.00 C

HETATM 502 C ATT A 57 2.207 2.683 -0.580 0.78810546E+000 1.00 C

HETATM 503 C ATT A 57 2.302 2.683 -0.611 0.78724915E+000 1.00 C

HETATM 504 C ATT A 57 2.397 2.683 -0.580 0.78818305E+000 1.00 C

HETATM 505 C ATT A 57 2.334 2.746 -0.643 0.78824230E+000 1.00 C

HETATM 506 C ATT A 57 2.270 2.746 -0.643 0.78810646E+000 1.00 C

HETATM 507 C ATT A 57 2.397 2.778 -0.643 0.78844493E+000 1.00 C

HETATM 508 C ATT A 117 1.667 3.699 -0.865 0.87770609E+000 1.00 C

HETATM 509 C ATT A 57 2.207 2.778 -0.643 0.78812557E+000 1.00 C

HETATM 510 C ATT A 57 2.492 2.778 -0.580 0.78852893E+000 1.00 C

HETATM 511 C ATT A 57 2.111 2.873 -0.611 0.78804071E+000 1.00 C

HETATM 512 C ATT A 117 1.667 3.731 -0.802 0.87771374E+000 1.00 C

HETATM 513 C ATT A 57 2.270 2.905 -0.675 0.78852111E+000 1.00 C

HETATM 514 C ATT A 57 2.334 2.842 -0.675 0.78850141E+000 1.00 C

HETATM 515 C ATT A 57 2.429 2.842 -0.643 0.78850355E+000 1.00 C

HETATM 516 C ATT A 57 2.492 2.873 -0.611 0.78787410E+000 1.00 C

HETATM 517 C ATT A 63 -1.572 3.127 -0.611 0.78805891E+000 1.00 C

HETATM 518 C ATT A 63 -1.476 3.096 -0.580 0.78822882E+000 1.00 C

HETATM 519 C ATT A 63 -1.381 3.127 -0.643 0.78806229E+000 1.00 C

HETATM 520 C ATT A 57 2.334 2.905 -0.675 0.78858149E+000 1.00 C

HETATM 521 C ATT A 57 2.175 2.937 -0.643 0.78844579E+000 1.00 C

HETATM 522 C ATT A 57 2.429 2.937 -0.643 0.78837056E+000 1.00 C

HETATM 523 C ATT A 63 -1.635 3.191 -0.643 0.78819819E+000 1.00 C

HETATM 524 C ATT A 63 -1.381 3.096 -0.516 0.78847824E+000 1.00 C

HETATM 525 C ATT A 63 -1.318 3.127 -0.580 0.78838224E+000 1.00 C

HETATM 526 C ATT A 63 -1.572 3.191 -0.707 0.78815312E+000 1.00 C

HETATM 527 C ATT A 63 -1.286 3.191 -0.675 0.78778714E+000 1.00 C

HETATM 528 C ATT A 57 2.238 3.000 -0.643 0.78858579E+000 1.00 C

HETATM 529 C ATT A 57 2.365 3.000 -0.643 0.78838468E+000 1.00 C

HETATM 530 C ATT A 63 -1.222 3.254 -0.643 0.78810078E+000 1.00 C

HETATM 531 C ATT A 63 -1.699 3.286 -0.643 0.78844145E+000 1.00 C

HETATM 532 C ATT A 63 -1.508 3.191 -0.738 0.78808990E+000 1.00 C

HETATM 533 C ATT A 105 -2.905 0.111 -2.516 0.78835077E+000 1.00 C

HETATM 534 C ATT A 63 -1.413 3.191 -0.738 0.78809229E+000 1.00 C

HETATM 535 C ATT A 104 2.905 -0.111 -2.516 0.78837103E+000 1.00 C

HETATM 536 C ATT A 57 2.302 3.064 -0.611 0.78830671E+000 1.00 C

HETATM 537 C ATT A 63 -1.635 3.254 -0.707 0.78838172E+000 1.00 C

HETATM 538 C ATT A 63 -1.381 3.254 -0.770 0.78809116E+000 1.00 C

HETATM 539 C ATT A 57 2.143 3.064 -0.548 0.78835727E+000 1.00 C

HETATM 540 C ATT A 63 -1.572 3.286 -0.770 0.78837734E+000 1.00 C

HETATM 541 C ATT A 63 -1.667 3.318 -0.707 0.78846906E+000 1.00 C

HETATM 542 C ATT A 63 -1.508 3.350 -0.802 0.78854101E+000 1.00 C

HETATM 543 C ATT A 63 -1.318 3.318 -0.770 0.78830074E+000 1.00 C

HETATM 544 C ATT A 63 -1.254 3.381 -0.738 0.78732806E+000 1.00 C

HETATM 545 C ATT A 63 -1.191 3.318 -0.611 0.78793580E+000 1.00 C

HETATM 546 C ATT A 63 -1.413 3.318 -0.802 0.78841192E+000 1.00 C

HETATM 547 C ATT A 63 -1.191 3.381 -0.643 0.78803652E+000 1.00 C

HETATM 548 C ATT A 63 -1.730 3.350 -0.580 0.78855123E+000 1.00 C

HETATM 549 C ATT A 63 -1.635 3.413 -0.738 0.78841851E+000 1.00 C

HETATM 550 C ATT A 63 -1.413 3.413 -0.802 0.78856363E+000 1.00 C

HETATM 551 C ATT A 63 -1.318 3.413 -0.770 0.78853158E+000 1.00 C

HETATM 552 C ATT A 63 -1.572 3.445 -0.770 0.78824678E+000 1.00 C

HETATM 553 C ATT A 63 -1.508 3.413 -0.802 0.78854069E+000 1.00 C

HETATM 554 C ATT A 63 -1.222 3.445 -0.675 0.78847054E+000 1.00 C

HETATM 555 C ATT A 63 -1.699 3.445 -0.643 0.78809316E+000 1.00 C

HETATM 556 C ATT A 63 -1.191 3.445 -0.611 0.78837405E+000 1.00 C

HETATM 557 C ATT A 63 -1.508 3.508 -0.770 0.78819620E+000 1.00 C

HETATM 558 C ATT A 63 -1.413 3.508 -0.770 0.78837685E+000 1.00 C

HETATM 559 C ATT A 63 -1.349 3.477 -0.770 0.78855569E+000 1.00 C

HETATM 560 C ATT A 63 -1.254 3.508 -0.675 0.78854205E+000 1.00 C

HETATM 561 C ATT A 63 -1.603 3.540 -0.707 0.78741722E+000 1.00 C

HETATM 562 C ATT A 63 -1.445 3.572 -0.738 0.78710464E+000 1.00 C

HETATM 563 C ATT A 63 -1.445 3.667 -0.516 0.78605001E+000 1.00 C

HETATM 564 C ATT A 63 -1.699 3.508 -0.580 0.78785876E+000 1.00 C

HETATM 565 C ATT A 63 -1.445 3.635 -0.643 0.78732454E+000 1.00 C

HETATM 566 C ATT A 104 2.746 -0.333 -2.389 0.78724768E+000 1.00 C

HETATM 567 C ATT A 104 2.778 -0.397 -2.485 0.78809830E+000 1.00 C

HETATM 568 C ATT A 104 3.286 -0.206 -2.453 0.78771264E+000 1.00 C

HETATM 569 C ATT A 105 -2.810 0.175 -2.453 0.78808506E+000 1.00 C

HETATM 570 C ATT A 104 2.842 -0.143 -2.485 0.78808680E+000 1.00 C

HETATM 571 C ATT A 105 -3.286 0.206 -2.453 0.78771495E+000 1.00 C

HETATM 572 C ATT A 105 -2.778 0.270 -2.485 0.78805012E+000 1.00 C

HETATM 573 C ATT A 105 -2.778 0.397 -2.485 0.78810352E+000 1.00 C

HETATM 574 C ATT A 105 -2.746 0.333 -2.389 0.78716261E+000 1.00 C

HETATM 575 C ATT A 105 -3.159 0.587 -2.421 0.78841374E+000 1.00 C

HETATM 576 C ATT A 105 -3.032 0.619 -2.389 0.78812472E+000 1.00 C

HETATM 577 C ATT A 104 2.969 -0.587 -2.485 0.78838354E+000 1.00 C

HETATM 578 C ATT A 105 -3.159 0.079 -2.453 0.78846159E+000 1.00 C

HETATM 579 C ATT A 104 3.159 -0.079 -2.453 0.78846378E+000 1.00 C

HETATM 580 C ATT A 105 -2.873 0.556 -2.453 0.78822731E+000 1.00 C

HETATM 581 C ATT A 105 -2.969 0.587 -2.485 0.78836630E+000 1.00 C

HETATM 582 C ATT A 104 3.032 -0.619 -2.389 0.78804954E+000 1.00 C

HETATM 583 C ATT A 104 2.873 -0.556 -2.453 0.78822348E+000 1.00 C

HETATM 584 C ATT A 104 3.254 -0.524 -2.389 0.78774478E+000 1.00 C

HETATM 585 C ATT A 105 -3.064 0.048 -2.421 0.78845420E+000 1.00 C

HETATM 586 C ATT A 105 -3.223 0.111 -2.389 0.78838078E+000 1.00 C

HETATM 587 C ATT A 104 3.223 -0.111 -2.389 0.78838795E+000 1.00 C

HETATM 588 C ATT A 104 3.064 -0.048 -2.421 0.78846886E+000 1.00 C

HETATM 589 C ATT A 105 -3.254 0.524 -2.389 0.78784110E+000 1.00 C

HETATM 590 C ATT A 104 3.159 -0.587 -2.389 0.78843451E+000 1.00 C

HETATM 591 C ATT A 105 -2.905 0.079 -2.421 0.78816352E+000 1.00 C

HETATM 592 C ATT A 104 2.905 -0.079 -2.421 0.78818919E+000 1.00 C

HETATM 593 C ATT A 118 3.064 -0.397 -2.421 0.77575997E+000 1.00 C

HETATM 594 C ATT A 118 3.000 -0.270 -2.421 0.77603476E+000 1.00 C

HETATM 595 C ATT A 119 3.032 -0.333 -2.389 0.99527358E+000 1.00 C

HETATM 596 C ATT A 105 -2.810 0.175 -2.326 0.78819739E+000 1.00 C

HETATM 597 C ATT A 120 -3.032 0.333 -2.389 0.99536541E+000 1.00 C

HETATM 598 C ATT A 121 -3.000 0.270 -2.421 0.77615440E+000 1.00 C

HETATM 599 C ATT A 121 -3.064 0.397 -2.421 0.77552364E+000 1.00 C

HETATM 600 C ATT A 104 2.778 -0.206 -2.389 0.78793830E+000 1.00 C

HETATM 601 C ATT A 104 2.810 -0.175 -2.326 0.78818967E+000 1.00 C

HETATM 602 C ATT A 18 1.222 -3.540 -0.516 0.78853486E+000 1.00 C

HETATM 603 C ATT A 18 1.667 -3.572 -0.516 0.78671550E+000 1.00 C

HETATM 604 C ATT A 18 1.191 -3.477 -0.548 0.78838279E+000 1.00 C

HETATM 605 C ATT A 19 -2.365 -3.127 -0.516 0.78753487E+000 1.00 C

HETATM 606 C ATT A 19 -2.207 -3.096 -0.548 0.78839674E+000 1.00 C

HETATM 607 C ATT A 19 -2.588 -2.873 -0.389 0.78812132E+000 1.00 C

HETATM 608 C ATT A 19 -2.080 -2.969 -0.548 0.78828240E+000 1.00 C

HETATM 609 C ATT A 18 1.254 -3.159 -0.516 0.78747500E+000 1.00 C

HETATM 610 C ATT A 19 -2.556 -2.842 -0.516 0.78842727E+000 1.00 C

HETATM 611 C ATT A 19 -2.048 -2.778 -0.484 0.78818629E+000 1.00 C

HETATM 612 C ATT A 19 -2.302 -2.619 -0.516 0.78810776E+000 1.00 C

HETATM 613 C ATT A 118 3.000 -0.397 -2.389 0.77605047E+000 1.00 C

HETATM 614 C ATT A 118 3.064 -0.365 -2.326 0.77589817E+000 1.00 C

HETATM 615 C ATT A 122 3.064 -0.492 1.325 0.78797052E+000 1.00 C

HETATM 616 C ATT A 122 3.127 -0.333 1.325 0.78796993E+000 1.00 C

HETATM 617 C ATT A 122 3.191 -0.492 1.325 0.78807234E+000 1.00 C

HETATM 618 C ATT A 122 3.032 -0.429 1.325 0.78795087E+000 1.00 C

HETATM 619 C ATT A 122 3.064 -0.365 1.325 0.78810332E+000 1.00 C

HETATM 620 C ATT A 122 3.191 -0.365 1.325 0.78814906E+000 1.00 C

HETATM 621 C ATT A 121 -3.064 0.365 -2.326 0.77620354E+000 1.00 C

HETATM 622 C ATT A 121 -3.000 0.397 -2.389 0.77593777E+000 1.00 C

HETATM 623 C ATT A 123 -3.127 0.333 1.325 0.78796207E+000 1.00 C

HETATM 624 C ATT A 123 -3.191 0.365 1.325 0.78814166E+000 1.00 C

HETATM 625 C ATT A 123 -3.064 0.365 1.325 0.78810186E+000 1.00 C

HETATM 626 C ATT A 123 -3.191 0.460 1.325 0.78805464E+000 1.00 C

HETATM 627 C ATT A 105 -2.842 0.524 -2.326 0.78809928E+000 1.00 C

HETATM 628 C ATT A 123 -3.032 0.429 1.325 0.78794822E+000 1.00 C

HETATM 629 C ATT A 123 -3.064 0.492 1.325 0.78796311E+000 1.00 C

HETATM 630 C ATT A 57 2.302 2.619 -0.516 0.78810633E+000 1.00 C

HETATM 631 C ATT A 57 2.048 2.778 -0.484 0.78818686E+000 1.00 C

HETATM 632 C ATT A 57 2.524 2.746 -0.516 0.78839365E+000 1.00 C

HETATM 633 C ATT A 57 2.556 2.842 -0.516 0.78841770E+000 1.00 C

HETATM 634 C ATT A 57 2.588 2.873 -0.389 0.78810087E+000 1.00 C

HETATM 635 C ATT A 63 -1.254 3.159 -0.516 0.78749814E+000 1.00 C

HETATM 636 C ATT A 57 2.080 2.969 -0.548 0.78827904E+000 1.00 C

HETATM 637 C ATT A 57 2.207 3.096 -0.548 0.78839523E+000 1.00 C

HETATM 638 C ATT A 57 2.365 3.127 -0.516 0.78753432E+000 1.00 C

HETATM 639 C ATT A 63 -1.191 3.477 -0.548 0.78838464E+000 1.00 C

HETATM 640 C ATT A 104 2.842 -0.524 -2.326 0.78810750E+000 1.00 C

HETATM 641 C ATT A 63 -1.667 3.572 -0.516 0.78669572E+000 1.00 C

HETATM 642 C ATT A 63 -1.222 3.540 -0.516 0.78853456E+000 1.00 C

HETATM 643 C ATT A 105 -2.778 0.206 -2.389 0.78787305E+000 1.00 C

HETATM 644 C ATT A 105 -3.159 0.587 -2.358 0.78844314E+000 1.00 C

HETATM 645 C ATT A 122 3.000 -0.333 1.357 0.78819943E+000 1.00 C

HETATM 646 C ATT A 122 3.254 -0.333 1.357 0.78826477E+000 1.00 C

HETATM 647 C ATT A 123 -3.254 0.333 1.357 0.78824567E+000 1.00 C

HETATM 648 C ATT A 123 -3.000 0.333 1.357 0.78820363E+000 1.00 C

HETATM 649 C ATT A 18 1.667 -3.191 -0.580 0.78817524E+000 1.00 C

HETATM 650 C ATT A 19 -2.016 -2.905 -0.389 0.78809191E+000 1.00 C

HETATM 651 C ATT A 19 -2.524 -2.746 -0.516 0.78841428E+000 1.00 C

HETATM 652 C ATT A 19 -2.175 -2.651 -0.516 0.78826681E+000 1.00 C

HETATM 653 C ATT A 57 2.175 2.651 -0.516 0.78826643E+000 1.00 C

HETATM 654 C ATT A 57 2.016 2.905 -0.389 0.78809250E+000 1.00 C

HETATM 655 C ATT A 63 -1.667 3.191 -0.580 0.78817680E+000 1.00 C

HETATM 656 C ATT A 104 2.937 -0.587 -2.326 0.78815355E+000 1.00 C

HETATM 657 C ATT A 104 3.096 -0.587 -2.294 0.78809549E+000 1.00 C

HETATM 658 C ATT A 104 3.223 -0.524 -2.294 0.78844461E+000 1.00 C

HETATM 659 C ATT A 104 2.778 -0.397 -2.294 0.78832418E+000 1.00 C

HETATM 660 C ATT A 118 3.064 -0.302 -2.326 0.77581814E+000 1.00 C

HETATM 661 C ATT A 104 2.778 -0.270 -2.294 0.78837281E+000 1.00 C

HETATM 662 C ATT A 118 3.000 -0.270 -2.358 0.77526415E+000 1.00 C

HETATM 663 C ATT A 104 3.254 -0.175 -2.294 0.78846386E+000 1.00 C

HETATM 664 C ATT A 104 3.191 -0.111 -2.294 0.78847140E+000 1.00 C

HETATM 665 C ATT A 105 -3.191 0.111 -2.294 0.78847151E+000 1.00 C

HETATM 666 C ATT A 105 -3.254 0.175 -2.294 0.78845493E+000 1.00 C

HETATM 667 C ATT A 105 -2.778 0.270 -2.294 0.78837513E+000 1.00 C

HETATM 668 C ATT A 105 -2.778 0.397 -2.294 0.78832309E+000 1.00 C

HETATM 669 C ATT A 105 -3.223 0.524 -2.294 0.78843044E+000 1.00 C

HETATM 670 C ATT A 105 -2.937 0.587 -2.326 0.78814434E+000 1.00 C

HETATM 671 C ATT A 122 3.032 -0.587 1.389 0.78779675E+000 1.00 C

HETATM 672 C ATT A 122 3.223 -0.587 1.389 0.78816550E+000 1.00 C

HETATM 673 C ATT A 122 3.000 -0.524 1.357 0.78781473E+000 1.00 C

HETATM 674 C ATT A 122 3.286 -0.524 1.389 0.78812905E+000 1.00 C

HETATM 675 C ATT A 122 3.318 -0.460 1.389 0.78855385E+000 1.00 C

HETATM 676 C ATT A 122 3.127 -0.270 1.357 0.78804865E+000 1.00 C

HETATM 677 C ATT A 123 -3.127 0.270 1.357 0.78804615E+000 1.00 C

HETATM 678 C ATT A 123 -3.318 0.397 1.389 0.78854350E+000 1.00 C

HETATM 679 C ATT A 123 -3.318 0.460 1.389 0.78855192E+000 1.00 C

HETATM 680 C ATT A 123 -3.286 0.524 1.389 0.78818319E+000 1.00 C

HETATM 681 C ATT A 123 -3.000 0.524 1.357 0.78781391E+000 1.00 C

HETATM 682 C ATT A 123 -3.223 0.587 1.389 0.78820228E+000 1.00 C

HETATM 683 C ATT A 123 -3.032 0.587 1.389 0.78780346E+000 1.00 C

HETATM 684 C ATT A 104 3.032 -0.587 -2.262 0.78796123E+000 1.00 C

HETATM 685 C ATT A 104 3.159 -0.556 -2.262 0.78830924E+000 1.00 C

HETATM 686 C ATT A 104 2.969 -0.556 -2.231 0.78805850E+000 1.00 C

HETATM 687 C ATT A 104 2.842 -0.460 -2.231 0.78827720E+000 1.00 C

HETATM 688 C ATT A 104 3.254 -0.460 -2.262 0.78843336E+000 1.00 C

HETATM 689 C ATT A 118 3.000 -0.333 -2.326 0.77564218E+000 1.00 C

HETATM 690 C ATT A 104 2.810 -0.270 -2.231 0.78846094E+000 1.00 C

HETATM 691 C ATT A 104 3.254 -0.238 -2.231 0.78851293E+000 1.00 C

HETATM 692 C ATT A 104 3.159 -0.206 -2.167 0.78826284E+000 1.00 C

HETATM 693 C ATT A 104 2.905 -0.111 -2.262 0.78802135E+000 1.00 C

HETATM 694 C ATT A 104 3.127 -0.111 -2.231 0.78823701E+000 1.00 C

HETATM 695 C ATT A 104 3.000 -0.079 -2.262 0.78812166E+000 1.00 C

HETATM 696 C ATT A 104 3.064 -0.079 -2.262 0.78818186E+000 1.00 C

HETATM 697 C ATT A 105 -3.064 0.079 -2.262 0.78818855E+000 1.00 C

HETATM 698 C ATT A 105 -3.000 0.079 -2.262 0.78811971E+000 1.00 C

HETATM 699 C ATT A 105 -2.905 0.111 -2.262 0.78799435E+000 1.00 C

HETATM 700 C ATT A 105 -3.127 0.111 -2.231 0.78823877E+000 1.00 C

HETATM 701 C ATT A 121 -3.064 0.302 -2.326 0.77554257E+000 1.00 C

HETATM 702 C ATT A 105 -2.842 0.206 -2.231 0.78829914E+000 1.00 C

HETATM 703 C ATT A 105 -3.159 0.302 -2.135 0.78824187E+000 1.00 C

HETATM 704 C ATT A 105 -3.254 0.238 -2.231 0.78851302E+000 1.00 C

HETATM 705 C ATT A 105 -2.810 0.270 -2.231 0.78845702E+000 1.00 C

HETATM 706 C ATT A 105 -3.254 0.429 -2.231 0.78843493E+000 1.00 C

HETATM 707 C ATT A 105 -2.842 0.460 -2.231 0.78828523E+000 1.00 C

HETATM 708 C ATT A 105 -3.159 0.556 -2.262 0.78835761E+000 1.00 C

HETATM 709 C ATT A 105 -2.969 0.492 -2.167 0.78809900E+000 1.00 C

HETATM 710 C ATT A 105 -3.032 0.587 -2.262 0.78803732E+000 1.00 C

HETATM 711 C ATT A 18 1.572 -3.635 -0.516 0.78698054E+000 1.00 C

HETATM 712 C ATT A 124 1.413 -3.413 -0.580 0.77593472E+000 1.00 C

HETATM 713 C ATT A 124 1.508 -3.381 -0.580 0.77616559E+000 1.00 C

HETATM 714 C ATT A 124 1.445 -3.318 -0.580 0.77578743E+000 1.00 C

HETATM 715 C ATT A 19 -2.461 -3.096 -0.484 0.78706038E+000 1.00 C

HETATM 716 C ATT A 19 -2.556 -2.969 -0.484 0.78768092E+000 1.00 C

HETATM 717 C ATT A 19 -2.080 -3.032 -0.484 0.78841813E+000 1.00 C

HETATM 718 C ATT A 18 1.191 -3.254 -0.516 0.78795449E+000 1.00 C

HETATM 719 C ATT A 19 -2.111 -2.683 -0.484 0.78836345E+000 1.00 C

HETATM 720 C ATT A 19 -2.429 -2.651 -0.516 0.78802740E+000 1.00 C

HETATM 721 C ATT A 122 3.127 -0.619 1.389 0.78819550E+000 1.00 C

HETATM 722 C ATT A 57 2.429 2.651 -0.516 0.78800894E+000 1.00 C

HETATM 723 C ATT A 57 2.111 2.683 -0.484 0.78836350E+000 1.00 C

HETATM 724 C ATT A 104 3.096 -0.556 -2.231 0.78818654E+000 1.00 C

HETATM 725 C ATT A 104 2.969 -0.492 -2.167 0.78808507E+000 1.00 C

HETATM 726 C ATT A 104 3.223 -0.429 -2.199 0.78843295E+000 1.00 C

HETATM 727 C ATT A 104 2.842 -0.397 -2.199 0.78839821E+000 1.00 C

HETATM 728 C ATT A 104 3.254 -0.333 -2.199 0.78799947E+000 1.00 C

HETATM 729 C ATT A 104 2.842 -0.206 -2.231 0.78828907E+000 1.00 C

HETATM 730 C ATT A 63 -1.191 3.254 -0.516 0.78796178E+000 1.00 C

HETATM 731 C ATT A 57 2.556 2.969 -0.484 0.78767502E+000 1.00 C

HETATM 732 C ATT A 104 2.937 -0.143 -2.199 0.78803036E+000 1.00 C

HETATM 733 C ATT A 104 3.032 -0.111 -2.199 0.78710600E+000 1.00 C

HETATM 734 C ATT A 57 2.080 3.032 -0.484 0.78841453E+000 1.00 C

HETATM 735 C ATT A 57 2.461 3.096 -0.484 0.78706236E+000 1.00 C

HETATM 736 C ATT A 123 -3.127 0.619 1.389 0.78819373E+000 1.00 C

HETATM 737 C ATT A 125 -1.445 3.318 -0.580 0.77577865E+000 1.00 C

HETATM 738 C ATT A 125 -1.508 3.381 -0.580 0.77615286E+000 1.00 C

HETATM 739 C ATT A 125 -1.413 3.413 -0.580 0.77587787E+000 1.00 C

HETATM 740 C ATT A 105 -3.032 0.111 -2.199 0.78709989E+000 1.00 C

HETATM 741 C ATT A 105 -2.937 0.270 -2.135 0.78815986E+000 1.00 C

HETATM 742 C ATT A 105 -3.254 0.333 -2.199 0.78810731E+000 1.00 C

HETATM 743 C ATT A 105 -2.842 0.397 -2.199 0.78838590E+000 1.00 C

HETATM 744 C ATT A 105 -3.127 0.524 -2.199 0.78814939E+000 1.00 C

HETATM 745 C ATT A 105 -2.969 0.556 -2.231 0.78807713E+000 1.00 C

HETATM 746 C ATT A 63 -1.572 3.635 -0.516 0.78697302E+000 1.00 C

HETATM 747 C ATT A 104 3.032 -0.460 -2.135 0.78790744E+000 1.00 C

HETATM 748 C ATT A 104 3.096 -0.492 -2.167 0.78808517E+000 1.00 C

HETATM 749 C ATT A 104 3.159 -0.460 -2.167 0.78819751E+000 1.00 C

HETATM 750 C ATT A 104 2.937 -0.397 -2.135 0.78823835E+000 1.00 C

HETATM 751 C ATT A 104 3.032 -0.333 -2.104 0.78788089E+000 1.00 C

HETATM 752 C ATT A 104 3.159 -0.302 -2.135 0.78823903E+000 1.00 C

HETATM 753 C ATT A 104 2.873 -0.270 -2.167 0.78844280E+000 1.00 C

HETATM 754 C ATT A 104 3.032 -0.206 -2.135 0.78811813E+000 1.00 C

HETATM 755 C ATT A 105 -3.032 0.333 -2.104 0.78794517E+000 1.00 C

HETATM 756 C ATT A 105 -3.032 0.206 -2.135 0.78811855E+000 1.00 C

HETATM 757 C ATT A 105 -2.873 0.270 -2.167 0.78844422E+000 1.00 C

HETATM 758 C ATT A 105 -2.905 0.333 -2.135 0.78810777E+000 1.00 C

HETATM 759 C ATT A 105 -3.159 0.365 -2.135 0.78823263E+000 1.00 C

HETATM 760 C ATT A 105 -3.159 0.460 -2.167 0.78824154E+000 1.00 C

HETATM 761 C ATT A 105 -2.937 0.397 -2.135 0.78821723E+000 1.00 C

HETATM 762 C ATT A 105 -3.032 0.460 -2.135 0.78797471E+000 1.00 C

HETATM 763 C ATT A 122 3.286 -0.587 1.421 0.78837246E+000 1.00 C

HETATM 764 C ATT A 122 2.905 -0.397 1.421 0.78856408E+000 1.00 C

HETATM 765 C ATT A 122 3.096 -0.206 1.421 0.78802826E+000 1.00 C

HETATM 766 C ATT A 122 3.159 -0.206 1.421 0.78812869E+000 1.00 C

HETATM 767 C ATT A 123 -3.159 0.206 1.421 0.78813122E+000 1.00 C

HETATM 768 C ATT A 123 -3.096 0.206 1.421 0.78802592E+000 1.00 C

HETATM 769 C ATT A 123 -2.905 0.397 1.421 0.78856627E+000 1.00 C

HETATM 770 C ATT A 18 1.159 -3.381 -0.516 0.78643998E+000 1.00 C

HETATM 771 C ATT A 124 1.476 -3.445 -0.548 0.77649713E+000 1.00 C

HETATM 772 C ATT A 19 -2.143 -3.096 -0.484 0.78852294E+000 1.00 C

HETATM 773 C ATT A 19 -2.492 -3.096 -0.389 0.78649238E+000 1.00 C

HETATM 774 C ATT A 104 2.937 -0.270 -2.135 0.78818403E+000 1.00 C

HETATM 775 C ATT A 57 2.524 2.715 -0.453 0.78844735E+000 1.00 C

HETATM 776 C ATT A 63 -1.159 3.381 -0.516 0.78644885E+000 1.00 C

HETATM 777 C ATT A 57 2.492 3.096 -0.389 0.78647447E+000 1.00 C

HETATM 778 C ATT A 57 2.143 3.096 -0.484 0.78851838E+000 1.00 C

HETATM 779 C ATT A 125 -1.476 3.445 -0.548 0.77647968E+000 1.00 C

HETATM 780 C ATT A 122 3.096 -0.683 1.484 0.78824075E+000 1.00 C

HETATM 781 C ATT A 122 2.969 -0.587 1.421 0.78797292E+000 1.00 C

HETATM 782 C ATT A 122 3.350 -0.397 1.421 0.78854451E+000 1.00 C

HETATM 783 C ATT A 123 -2.842 0.429 1.579 0.78832553E+000 1.00 C

HETATM 784 C ATT A 123 -3.286 0.587 1.421 0.78833417E+000 1.00 C

HETATM 785 C ATT A 123 -2.969 0.587 1.421 0.78797664E+000 1.00 C

HETATM 786 C ATT A 123 -3.096 0.683 1.484 0.78824714E+000 1.00 C

HETATM 787 C ATT A 126 1.445 -3.381 -0.516 0.96552906E+000 1.00 C

HETATM 788 C ATT A 19 -2.524 -2.715 -0.453 0.78843825E+000 1.00 C

HETATM 789 C ATT A 19 -2.397 -2.619 -0.453 0.78793598E+000 1.00 C

HETATM 790 C ATT A 57 2.556 2.778 -0.453 0.78828751E+000 1.00 C

HETATM 791 C ATT A 122 3.032 -0.651 1.452 0.78810094E+000 1.00 C

HETATM 792 C ATT A 122 3.159 -0.683 1.484 0.78840238E+000 1.00 C

HETATM 793 C ATT A 122 3.223 -0.651 1.452 0.78851836E+000 1.00 C

HETATM 794 C ATT A 122 2.842 -0.429 1.579 0.78831092E+000 1.00 C

HETATM 795 C ATT A 122 3.350 -0.524 1.452 0.78842041E+000 1.00 C

HETATM 796 C ATT A 127 -1.445 3.381 -0.516 0.96595500E+000 1.00 C

HETATM 797 C ATT A 122 2.937 -0.270 1.452 0.78835757E+000 1.00 C

HETATM 798 C ATT A 122 3.318 -0.270 1.452 0.78855300E+000 1.00 C

HETATM 799 C ATT A 123 -2.937 0.270 1.452 0.78835983E+000 1.00 C

HETATM 800 C ATT A 123 -3.318 0.270 1.452 0.78854664E+000 1.00 C

HETATM 801 C ATT A 123 -2.873 0.492 1.484 0.78841680E+000 1.00 C

HETATM 802 C ATT A 123 -3.350 0.524 1.452 0.78844217E+000 1.00 C

HETATM 803 C ATT A 123 -3.223 0.651 1.452 0.78851570E+000 1.00 C

HETATM 804 C ATT A 123 -3.159 0.683 1.484 0.78841218E+000 1.00 C

HETATM 805 C ATT A 123 -3.032 0.651 1.452 0.78810098E+000 1.00 C

HETATM 806 C ATT A 128 -0.111 -0.841 -1.659 0.99999953E+000 1.00 C

HETATM 807 C ATT A 129 0.111 0.841 -1.659 0.99999953E+000 1.00 C

HETATM 808 C ATT A 122 2.873 -0.492 1.484 0.78840883E+000 1.00 C

HETATM 809 C ATT A 122 2.873 -0.365 1.484 0.78856442E+000 1.00 C

HETATM 810 C ATT A 122 3.381 -0.365 1.484 0.78838307E+000 1.00 C

HETATM 811 C ATT A 122 3.191 -0.175 1.484 0.78822234E+000 1.00 C

HETATM 812 C ATT A 122 3.064 -0.175 1.484 0.78795385E+000 1.00 C

HETATM 813 C ATT A 123 -3.191 0.175 1.484 0.78822574E+000 1.00 C

HETATM 814 C ATT A 123 -3.064 0.175 1.484 0.78794239E+000 1.00 C

HETATM 815 C ATT A 124 1.381 -3.350 -0.516 0.77562464E+000 1.00 C

HETATM 816 C ATT A 124 1.508 -3.413 -0.484 0.77617349E+000 1.00 C

HETATM 817 C ATT A 124 1.508 -3.318 -0.516 0.77601601E+000 1.00 C

HETATM 818 C ATT A 123 -2.873 0.365 1.484 0.78855934E+000 1.00 C

HETATM 819 C ATT A 18 1.667 -3.191 -0.484 0.78818401E+000 1.00 C

HETATM 820 C ATT A 123 -3.381 0.365 1.484 0.78838825E+000 1.00 C

HETATM 821 C ATT A 123 -3.413 0.429 1.579 0.78766483E+000 1.00 C

HETATM 822 C ATT A 19 -2.461 -2.651 -0.453 0.78820994E+000 1.00 C

HETATM 823 C ATT A 57 2.397 2.619 -0.453 0.78794974E+000 1.00 C

HETATM 824 C ATT A 57 2.461 2.651 -0.453 0.78821560E+000 1.00 C

HETATM 825 C ATT A 63 -1.667 3.191 -0.484 0.78818210E+000 1.00 C

HETATM 826 C ATT A 63 -1.508 3.096 -0.484 0.78829082E+000 1.00 C

HETATM 827 C ATT A 125 -1.381 3.350 -0.516 0.77557867E+000 1.00 C

HETATM 828 C ATT A 125 -1.508 3.318 -0.516 0.77604312E+000 1.00 C

HETATM 829 C ATT A 125 -1.508 3.413 -0.484 0.77617391E+000 1.00 C

HETATM 830 C ATT A 122 2.937 -0.619 1.516 0.78807585E+000 1.00 C

HETATM 831 C ATT A 122 3.413 -0.429 1.579 0.78767207E+000 1.00 C

HETATM 832 C ATT A 123 -2.905 0.587 1.516 0.78807510E+000 1.00 C

HETATM 833 C ATT A 18 1.349 -3.635 -0.484 0.78809237E+000 1.00 C

HETATM 834 C ATT A 18 1.699 -3.508 -0.484 0.78789709E+000 1.00 C

HETATM 835 C ATT A 18 1.318 -3.127 -0.484 0.78847756E+000 1.00 C

HETATM 836 C ATT A 19 -2.556 -2.778 -0.453 0.78825652E+000 1.00 C

HETATM 837 C ATT A 19 -2.048 -2.746 -0.421 0.78833323E+000 1.00 C

HETATM 838 C ATT A 57 2.048 2.746 -0.421 0.78833268E+000 1.00 C

HETATM 839 C ATT A 63 -1.318 3.127 -0.484 0.78846926E+000 1.00 C

HETATM 840 C ATT A 122 3.223 -0.683 1.516 0.78850023E+000 1.00 C

HETATM 841 C ATT A 122 3.318 -0.619 1.516 0.78839302E+000 1.00 C

HETATM 842 C ATT A 122 3.350 -0.270 1.516 0.78841155E+000 1.00 C

HETATM 843 C ATT A 63 -1.191 3.477 -0.484 0.78841022E+000 1.00 C

HETATM 844 C ATT A 122 3.000 -0.175 1.548 0.78807295E+000 1.00 C

HETATM 845 C ATT A 122 3.254 -0.175 1.548 0.78853875E+000 1.00 C

HETATM 846 C ATT A 63 -1.699 3.508 -0.484 0.78790036E+000 1.00 C

HETATM 847 C ATT A 123 -3.254 0.175 1.548 0.78853740E+000 1.00 C

HETATM 848 C ATT A 123 -3.000 0.175 1.548 0.78807555E+000 1.00 C

HETATM 849 C ATT A 63 -1.349 3.635 -0.484 0.78809254E+000 1.00 C

HETATM 850 C ATT A 122 3.159 -0.143 1.611 0.78842977E+000 1.00 C

HETATM 851 C ATT A 123 -3.350 0.270 1.516 0.78842722E+000 1.00 C

HETATM 852 C ATT A 123 -3.318 0.619 1.516 0.78840557E+000 1.00 C

HETATM 853 C ATT A 122 3.032 -0.683 1.516 0.78810792E+000 1.00 C

HETATM 854 C ATT A 123 -3.159 0.143 1.611 0.78842943E+000 1.00 C

HETATM 855 C ATT A 123 -3.032 0.683 1.516 0.78810668E+000 1.00 C

HETATM 856 C ATT A 18 1.191 -3.477 -0.484 0.78840986E+000 1.00 C

HETATM 857 C ATT A 19 -2.111 -3.096 -0.389 0.78827466E+000 1.00 C

HETATM 858 C ATT A 130 -2.302 -2.937 -0.453 0.77049826E+000 1.00 C

HETATM 859 C ATT A 131 -2.365 -2.905 -0.421 0.77468037E+000 1.00 C

HETATM 860 C ATT A 131 -2.365 -2.842 -0.421 0.77580857E+000 1.00 C

HETATM 861 C ATT A 131 -2.270 -2.810 -0.421 0.77552294E+000 1.00 C

HETATM 862 C ATT A 132 2.334 2.842 -0.453 0.77578326E+000 1.00 C

HETATM 863 C ATT A 133 2.302 2.937 -0.453 0.77033077E+000 1.00 C

HETATM 864 C ATT A 132 2.365 2.905 -0.421 0.77492132E+000 1.00 C

HETATM 865 C ATT A 57 2.111 3.096 -0.389 0.78829561E+000 1.00 C

HETATM 866 C ATT A 123 -2.873 0.302 1.548 0.78832946E+000 1.00 C

HETATM 867 C ATT A 123 -3.127 0.714 1.611 0.78803723E+000 1.00 C

HETATM 868 C ATT A 18 1.318 -3.604 -0.421 0.78836762E+000 1.00 C

HETATM 869 C ATT A 18 1.222 -3.508 -0.421 0.78840758E+000 1.00 C

HETATM 870 C ATT A 18 1.699 -3.477 -0.421 0.78823437E+000 1.00 C

HETATM 871 C ATT A 18 1.730 -3.381 -0.453 0.78843401E+000 1.00 C

HETATM 872 C ATT A 18 1.191 -3.350 -0.421 0.78806506E+000 1.00 C

HETATM 873 C ATT A 18 1.730 -3.318 -0.484 0.78849671E+000 1.00 C

HETATM 874 C ATT A 18 1.191 -3.286 -0.453 0.78810736E+000 1.00 C

HETATM 875 C ATT A 18 1.222 -3.223 -0.453 0.78824184E+000 1.00 C

HETATM 876 C ATT A 18 1.699 -3.254 -0.453 0.78822610E+000 1.00 C

HETATM 877 C ATT A 18 1.572 -3.127 -0.453 0.78800815E+000 1.00 C

HETATM 878 C ATT A 19 -2.556 -3.000 -0.421 0.78741100E+000 1.00 C

HETATM 879 C ATT A 122 3.127 -0.714 1.611 0.78805554E+000 1.00 C

HETATM 880 C ATT A 134 -2.302 -2.873 -0.389 0.99693081E+000 1.00 C

HETATM 881 C ATT A 130 -2.238 -2.905 -0.421 0.76908915E+000 1.00 C

HETATM 882 C ATT A 19 -2.080 -2.683 -0.389 0.78718949E+000 1.00 C

HETATM 883 C ATT A 19 -2.175 -2.619 -0.389 0.78846882E+000 1.00 C

HETATM 884 C ATT A 122 2.937 -0.206 1.611 0.78751600E+000 1.00 C

HETATM 885 C ATT A 122 3.318 -0.206 1.611 0.78790905E+000 1.00 C

HETATM 886 C ATT A 123 -3.318 0.206 1.611 0.78788355E+000 1.00 C

HETATM 887 C ATT A 123 -2.937 0.206 1.611 0.78757408E+000 1.00 C

HETATM 888 C ATT A 123 -3.254 0.683 1.579 0.78831231E+000 1.00 C

HETATM 889 C ATT A 57 2.175 2.619 -0.389 0.78847127E+000 1.00 C

HETATM 890 C ATT A 57 2.080 2.683 -0.389 0.78722535E+000 1.00 C

HETATM 891 C ATT A 135 2.302 2.873 -0.389 0.99696068E+000 1.00 C

HETATM 892 C ATT A 132 2.270 2.810 -0.421 0.77552272E+000 1.00 C

HETATM 893 C ATT A 133 2.238 2.905 -0.421 0.76875145E+000 1.00 C

HETATM 894 C ATT A 63 -1.572 3.127 -0.453 0.78799610E+000 1.00 C

HETATM 895 C ATT A 57 2.556 3.000 -0.421 0.78741427E+000 1.00 C

HETATM 896 C ATT A 63 -1.222 3.223 -0.453 0.78823940E+000 1.00 C

HETATM 897 C ATT A 63 -1.699 3.254 -0.453 0.78822115E+000 1.00 C

HETATM 898 C ATT A 63 -1.730 3.318 -0.484 0.78849746E+000 1.00 C

HETATM 899 C ATT A 63 -1.191 3.286 -0.453 0.78810915E+000 1.00 C

HETATM 900 C ATT A 63 -1.191 3.350 -0.421 0.78805978E+000 1.00 C

HETATM 901 C ATT A 63 -1.730 3.381 -0.453 0.78843448E+000 1.00 C

HETATM 902 C ATT A 63 -1.699 3.477 -0.421 0.78823359E+000 1.00 C

HETATM 903 C ATT A 63 -1.222 3.508 -0.421 0.78840942E+000 1.00 C

HETATM 904 C ATT A 63 -1.318 3.604 -0.421 0.78836563E+000 1.00 C

HETATM 905 C ATT A 122 3.254 -0.683 1.579 0.78833903E+000 1.00 C

HETATM 906 C ATT A 136 3.127 -0.429 1.516 0.77177294E+000 1.00 C

HETATM 907 C ATT A 137 -3.127 0.429 1.516 0.77151962E+000 1.00 C

HETATM 908 C ATT A 123 -3.000 0.683 1.611 0.78807561E+000 1.00 C

HETATM 909 C ATT A 138 1.413 -0.175 -1.183 0.99999962E+000 1.00 C

HETATM 910 C ATT A 139 -1.413 0.175 -1.183 0.99999962E+000 1.00 C

HETATM 911 C ATT A 18 1.413 -3.635 -0.421 0.78798044E+000 1.00 C

HETATM 912 C ATT A 18 1.286 -3.540 -0.357 0.78812631E+000 1.00 C

HETATM 913 C ATT A 18 1.191 -3.413 -0.421 0.78823589E+000 1.00 C

HETATM 914 C ATT A 18 1.699 -3.413 -0.389 0.78838839E+000 1.00 C

HETATM 915 C ATT A 124 1.476 -3.350 -0.453 0.77584471E+000 1.00 C

HETATM 916 C ATT A 18 1.699 -3.318 -0.389 0.78836833E+000 1.00 C

HETATM 917 C ATT A 18 1.254 -3.223 -0.389 0.78823153E+000 1.00 C

HETATM 918 C ATT A 18 1.349 -3.127 -0.421 0.78851491E+000 1.00 C

HETATM 919 C ATT A 18 1.413 -3.127 -0.389 0.78837167E+000 1.00 C

HETATM 920 C ATT A 18 1.508 -3.127 -0.389 0.78822244E+000 1.00 C

HETATM 921 C ATT A 131 -2.238 -2.905 -0.357 0.77599894E+000 1.00 C

HETATM 922 C ATT A 19 -2.556 -2.746 -0.389 0.78834658E+000 1.00 C

HETATM 923 C ATT A 19 -2.524 -2.715 -0.326 0.78841697E+000 1.00 C

HETATM 924 C ATT A 122 2.873 -0.556 1.579 0.78812045E+000 1.00 C

HETATM 925 C ATT A 122 3.381 -0.556 1.579 0.78781187E+000 1.00 C

HETATM 926 C ATT A 140 3.127 -0.429 1.611 0.97237425E+000 1.00 C

HETATM 927 C ATT A 141 3.191 -0.429 1.548 0.77474025E+000 1.00 C

HETATM 928 C ATT A 141 3.127 -0.365 1.548 0.77610225E+000 1.00 C

HETATM 929 C ATT A 142 -3.127 0.365 1.548 0.77610363E+000 1.00 C

HETATM 930 C ATT A 137 -3.191 0.429 1.548 0.77433719E+000 1.00 C

HETATM 931 C ATT A 123 -3.381 0.556 1.579 0.78780493E+000 1.00 C

HETATM 932 C ATT A 57 2.556 2.746 -0.389 0.78832494E+000 1.00 C

HETATM 933 C ATT A 132 2.238 2.905 -0.357 0.77588317E+000 1.00 C

HETATM 934 C ATT A 63 -1.349 3.127 -0.421 0.78851940E+000 1.00 C

HETATM 935 C ATT A 63 -1.508 3.127 -0.389 0.78822651E+000 1.00 C

HETATM 936 C ATT A 63 -1.413 3.127 -0.389 0.78836113E+000 1.00 C

HETATM 937 C ATT A 63 -1.254 3.223 -0.389 0.78822438E+000 1.00 C

HETATM 938 C ATT A 63 -1.699 3.318 -0.389 0.78837141E+000 1.00 C

HETATM 939 C ATT A 125 -1.476 3.350 -0.453 0.77592878E+000 1.00 C

HETATM 940 C ATT A 63 -1.699 3.413 -0.389 0.78838672E+000 1.00 C

HETATM 941 C ATT A 63 -1.191 3.413 -0.421 0.78823666E+000 1.00 C

HETATM 942 C ATT A 63 -1.286 3.540 -0.357 0.78813214E+000 1.00 C

HETATM 943 C ATT A 63 -1.413 3.635 -0.421 0.78798025E+000 1.00 C

HETATM 944 C ATT A 122 3.000 -0.683 1.611 0.78806941E+000 1.00 C

HETATM 945 C ATT A 141 3.096 -0.492 1.579 0.77586508E+000 1.00 C

HETATM 946 C ATT A 141 3.159 -0.492 1.579 0.77522938E+000 1.00 C

HETATM 947 C ATT A 143 -3.127 0.429 1.611 0.97339437E+000 1.00 C

HETATM 948 C ATT A 142 -3.159 0.492 1.579 0.77545569E+000 1.00 C

HETATM 949 C ATT A 142 -3.096 0.492 1.579 0.77585842E+000 1.00 C

HETATM 950 C ATT A 123 -2.873 0.556 1.579 0.78813029E+000 1.00 C

HETATM 951 C ATT A 123 -2.969 0.651 1.675 0.78816289E+000 1.00 C

HETATM 952 C ATT A 123 -2.905 0.587 1.675 0.78807944E+000 1.00 C

HETATM 953 C ATT A 18 1.603 -3.508 -0.326 0.78823158E+000 1.00 C

HETATM 954 C ATT A 19 -2.429 -3.127 -0.357 0.78701815E+000 1.00 C

HETATM 955 C ATT A 18 1.667 -3.381 -0.326 0.78733235E+000 1.00 C

HETATM 956 C ATT A 19 -2.556 -3.000 -0.357 0.78748775E+000 1.00 C

HETATM 957 C ATT A 19 -2.048 -3.000 -0.357 0.78820319E+000 1.00 C

HETATM 958 C ATT A 131 -2.334 -2.937 -0.357 0.77612717E+000 1.00 C

HETATM 959 C ATT A 19 -2.048 -2.746 -0.357 0.78834529E+000 1.00 C

HETATM 960 C ATT A 19 -2.429 -2.619 -0.389 0.78786115E+000 1.00 C

HETATM 961 C ATT A 57 2.429 2.619 -0.389 0.78784551E+000 1.00 C

HETATM 962 C ATT A 57 2.524 2.715 -0.326 0.78841189E+000 1.00 C

HETATM 963 C ATT A 57 2.048 2.746 -0.357 0.78835158E+000 1.00 C

HETATM 964 C ATT A 122 2.969 -0.651 1.675 0.78815301E+000 1.00 C

HETATM 965 C ATT A 141 3.064 -0.429 1.643 0.77608248E+000 1.00 C

HETATM 966 C ATT A 132 2.334 2.937 -0.357 0.77612443E+000 1.00 C

HETATM 967 C ATT A 57 2.048 3.000 -0.357 0.78818837E+000 1.00 C

HETATM 968 C ATT A 57 2.556 3.000 -0.357 0.78748385E+000 1.00 C

HETATM 969 C ATT A 142 -3.064 0.429 1.643 0.77615777E+000 1.00 C

HETATM 970 C ATT A 63 -1.635 3.223 -0.357 0.78773071E+000 1.00 C

HETATM 971 C ATT A 57 2.429 3.127 -0.357 0.78701989E+000 1.00 C

HETATM 972 C ATT A 63 -1.667 3.381 -0.326 0.78735151E+000 1.00 C

HETATM 973 C ATT A 63 -1.603 3.508 -0.326 0.78822954E+000 1.00 C

HETATM 974 C ATT A 122 3.000 -0.175 1.643 0.78811384E+000 1.00 C

HETATM 975 C ATT A 122 3.254 -0.175 1.643 0.78854220E+000 1.00 C

HETATM 976 C ATT A 141 3.191 -0.429 1.643 0.77627061E+000 1.00 C

HETATM 977 C ATT A 136 3.159 -0.365 1.643 0.77400460E+000 1.00 C

HETATM 978 C ATT A 123 -3.254 0.175 1.643 0.78854239E+000 1.00 C

HETATM 979 C ATT A 123 -3.000 0.175 1.643 0.78811071E+000 1.00 C

HETATM 980 C ATT A 137 -3.159 0.365 1.643 0.77404109E+000 1.00 C

HETATM 981 C ATT A 142 -3.191 0.429 1.643 0.77635982E+000 1.00 C

HETATM 982 C ATT A 19 -2.111 -3.064 -0.294 0.78847673E+000 1.00 C

HETATM 983 C ATT A 19 -2.556 -2.778 -0.326 0.78848750E+000 1.00 C

HETATM 984 C ATT A 19 -2.143 -2.651 -0.326 0.78848262E+000 1.00 C

HETATM 985 C ATT A 19 -2.207 -2.619 -0.326 0.78832686E+000 1.00 C

HETATM 986 C ATT A 132 2.238 2.842 -0.357 0.77436253E+000 1.00 C

HETATM 987 C ATT A 57 2.556 2.778 -0.326 0.78849596E+000 1.00 C

HETATM 988 C ATT A 122 3.223 -0.683 1.675 0.78839696E+000 1.00 C

HETATM 989 C ATT A 122 3.286 -0.651 1.675 0.78802688E+000 1.00 C

HETATM 990 C ATT A 122 3.064 -0.683 1.706 0.78842383E+000 1.00 C

HETATM 991 C ATT A 122 2.873 -0.492 1.706 0.78807662E+000 1.00 C

HETATM 992 C ATT A 122 2.873 -0.365 1.706 0.78800879E+000 1.00 C

HETATM 993 C ATT A 122 3.381 -0.365 1.706 0.78696279E+000 1.00 C

HETATM 994 C ATT A 122 3.381 -0.302 1.643 0.78780490E+000 1.00 C

HETATM 995 C ATT A 123 -2.873 0.302 1.643 0.78813932E+000 1.00 C

HETATM 996 C ATT A 123 -2.873 0.365 1.706 0.78797904E+000 1.00 C

HETATM 997 C ATT A 123 -2.873 0.492 1.706 0.78807052E+000 1.00 C

HETATM 998 C ATT A 123 -3.286 0.651 1.675 0.78801613E+000 1.00 C

HETATM 999 C ATT A 123 -3.223 0.683 1.675 0.78839513E+000 1.00 C

HETATM 1000 C ATT A 123 -3.064 0.683 1.706 0.78842622E+000 1.00 C

HETATM 1001 C ATT A 131 -2.302 -2.842 -0.326 0.77619644E+000 1.00 C

HETATM 1002 C ATT A 132 2.302 2.842 -0.326 0.77618156E+000 1.00 C

HETATM 1003 C ATT A 122 3.096 -0.651 1.770 0.78853411E+000 1.00 C

HETATM 1004 C ATT A 122 2.969 -0.587 1.770 0.78834292E+000 1.00 C

HETATM 1005 C ATT A 141 3.127 -0.429 1.675 0.77576511E+000 1.00 C

HETATM 1006 C ATT A 122 3.254 -0.238 1.770 0.78824866E+000 1.00 C

HETATM 1007 C ATT A 122 3.127 -0.175 1.738 0.78839051E+000 1.00 C

HETATM 1008 C ATT A 123 -3.223 0.175 1.706 0.78817703E+000 1.00 C

HETATM 1009 C ATT A 123 -3.127 0.175 1.738 0.78840561E+000 1.00 C

HETATM 1010 C ATT A 123 -3.254 0.238 1.770 0.78824704E+000 1.00 C

HETATM 1011 C ATT A 142 -3.127 0.429 1.675 0.77568155E+000 1.00 C

HETATM 1012 C ATT A 123 -2.969 0.587 1.770 0.78834647E+000 1.00 C

HETATM 1013 C ATT A 123 -3.096 0.651 1.770 0.78853521E+000 1.00 C

HETATM 1014 C ATT A 122 3.032 -0.556 1.833 0.78850680E+000 1.00 C

HETATM 1015 C ATT A 122 3.223 -0.556 1.833 0.78789787E+000 1.00 C

HETATM 1016 C ATT A 122 3.064 -0.492 1.865 0.78849417E+000 1.00 C

HETATM 1017 C ATT A 122 3.032 -0.429 1.865 0.78853129E+000 1.00 C

HETATM 1018 C ATT A 122 3.223 -0.397 1.865 0.78792892E+000 1.00 C

HETATM 1019 C ATT A 122 3.032 -0.302 1.833 0.78841944E+000 1.00 C

HETATM 1020 C ATT A 122 3.191 -0.206 1.770 0.78851002E+000 1.00 C

HETATM 1021 C ATT A 123 -3.191 0.206 1.770 0.78851176E+000 1.00 C

HETATM 1022 C ATT A 123 -3.032 0.302 1.833 0.78839999E+000 1.00 C

HETATM 1023 C ATT A 123 -3.286 0.397 1.833 0.78745097E+000 1.00 C

HETATM 1024 C ATT A 123 -3.223 0.397 1.865 0.78792628E+000 1.00 C

HETATM 1025 C ATT A 123 -3.032 0.397 1.865 0.78852631E+000 1.00 C

HETATM 1026 C ATT A 123 -3.223 0.556 1.833 0.78789535E+000 1.00 C

HETATM 1027 C ATT A 123 -3.032 0.556 1.833 0.78851454E+000 1.00 C

HETATM 1028 C ATT A 144 -0.206 -1.889 3.072 0.78804615E+000 1.00 C

HETATM 1029 C ATT A 144 -0.302 -1.889 3.072 0.78806748E+000 1.00 C

HETATM 1030 C ATT A 144 -0.333 -1.953 3.072 0.78764555E+000 1.00 C

HETATM 1031 C ATT A 144 -0.365 -2.048 3.040 0.78730417E+000 1.00 C

HETATM 1032 C ATT A 144 -0.048 -1.953 3.008 0.78826289E+000 1.00 C

HETATM 1033 C ATT A 144 -0.079 -1.857 3.008 0.78848427E+000 1.00 C

HETATM 1034 C ATT A 144 -0.333 -1.826 3.040 0.78833050E+000 1.00 C

HETATM 1035 C ATT A 144 -0.143 -1.794 3.008 0.78843657E+000 1.00 C

HETATM 1036 C ATT A 144 -0.270 -1.762 3.008 0.78855732E+000 1.00 C

HETATM 1037 C ATT A 122 2.969 -0.429 1.833 0.78838288E+000 1.00 C

HETATM 1038 C ATT A 122 3.286 -0.460 1.833 0.78734642E+000 1.00 C

HETATM 1039 C ATT A 122 3.286 -0.397 1.833 0.78745269E+000 1.00 C

HETATM 1040 C ATT A 122 3.096 -0.270 1.833 0.78854608E+000 1.00 C

HETATM 1041 C ATT A 122 3.159 -0.270 1.833 0.78847101E+000 1.00 C

HETATM 1042 C ATT A 123 -3.159 0.270 1.833 0.78846575E+000 1.00 C

HETATM 1043 C ATT A 123 -3.096 0.270 1.833 0.78854089E+000 1.00 C

HETATM 1044 C ATT A 123 -3.096 0.333 1.865 0.78854114E+000 1.00 C

HETATM 1045 C ATT A 123 -2.969 0.429 1.833 0.78837959E+000 1.00 C

HETATM 1046 C ATT A 123 -3.286 0.460 1.833 0.78734287E+000 1.00 C

HETATM 1047 C ATT A 145 0.206 1.889 3.072 0.78804626E+000 1.00 C

HETATM 1048 C ATT A 145 0.270 1.762 3.008 0.78855806E+000 1.00 C

HETATM 1049 C ATT A 145 0.143 1.794 3.008 0.78844014E+000 1.00 C

HETATM 1050 C ATT A 145 0.302 1.889 3.072 0.78807021E+000 1.00 C

HETATM 1051 C ATT A 145 0.333 1.826 3.040 0.78833934E+000 1.00 C

HETATM 1052 C ATT A 145 0.079 1.857 3.008 0.78848957E+000 1.00 C

HETATM 1053 C ATT A 145 0.048 1.953 3.008 0.78825332E+000 1.00 C

HETATM 1054 C ATT A 145 0.333 1.953 3.072 0.78765036E+000 1.00 C

HETATM 1055 C ATT A 145 0.365 2.048 3.040 0.78730402E+000 1.00 C

HETATM 1056 C ATT A 145 0.143 2.111 3.008 0.78691589E+000 1.00 C

HETATM 1057 C ATT A 122 3.096 -0.333 1.865 0.78854307E+000 1.00 C

HETATM 1058 C ATT A 144 -0.270 -2.175 2.976 0.78711132E+000 1.00 C

HETATM 1059 C ATT A 144 -0.206 -2.175 2.976 0.78720454E+000 1.00 C

HETATM 1060 C ATT A 144 -0.079 -2.111 2.976 0.78757012E+000 1.00 C

HETATM 1061 C ATT A 144 -0.460 -2.016 2.976 0.78801650E+000 1.00 C

HETATM 1062 C ATT A 144 -0.524 -1.953 2.849 0.78854536E+000 1.00 C

HETATM 1063 C ATT A 144 -0.460 -1.889 2.976 0.78833965E+000 1.00 C

HETATM 1064 C ATT A 144 -0.397 -1.794 2.976 0.78853896E+000 1.00 C

HETATM 1065 C ATT A 144 -0.365 -2.207 2.849 0.78815977E+000 1.00 C

HETATM 1066 C ATT A 144 -0.238 -2.238 2.786 0.78843098E+000 1.00 C

HETATM 1067 C ATT A 144 -0.143 -2.207 2.881 0.78803799E+000 1.00 C

HETATM 1068 C ATT A 144 -0.111 -2.207 2.786 0.78847998E+000 1.00 C

HETATM 1069 C ATT A 144 -0.460 -2.143 2.786 0.78830859E+000 1.00 C

HETATM 1070 C ATT A 144 -0.302 -2.207 2.913 0.78755393E+000 1.00 C

HETATM 1071 C ATT A 144 -0.492 -2.080 2.849 0.78843305E+000 1.00 C

HETATM 1072 C ATT A 144 -0.016 -2.111 2.849 0.78835050E+000 1.00 C

HETATM 1073 C ATT A 144 0.048 -1.953 2.786 0.78740266E+000 1.00 C

HETATM 1074 C ATT A 144 -0.016 -2.080 2.913 0.78838838E+000 1.00 C

HETATM 1075 C ATT A 144 -0.492 -2.016 2.913 0.78802089E+000 1.00 C

HETATM 1076 C ATT A 145 0.397 1.794 2.976 0.78853410E+000 1.00 C

HETATM 1077 C ATT A 146 -0.238 -2.016 2.849 0.77539475E+000 1.00 C

HETATM 1078 C ATT A 147 -0.238 -1.953 2.881 0.77236093E+000 1.00 C

HETATM 1079 C ATT A 144 0.016 -1.953 2.913 0.78853648E+000 1.00 C

HETATM 1080 C ATT A 145 0.460 1.889 2.976 0.78835642E+000 1.00 C

HETATM 1081 C ATT A 146 -0.302 -1.953 2.849 0.77573883E+000 1.00 C

HETATM 1082 C ATT A 145 0.492 1.953 2.945 0.78826447E+000 1.00 C

HETATM 1083 C ATT A 144 -0.492 -1.889 2.913 0.78827129E+000 1.00 C

HETATM 1084 C ATT A 145 0.460 2.016 2.976 0.78802657E+000 1.00 C

HETATM 1085 C ATT A 148 -0.238 -1.953 2.786 0.96122670E+000 1.00 C

HETATM 1086 C ATT A 144 -0.016 -1.826 2.913 0.78845456E+000 1.00 C

HETATM 1087 C ATT A 145 0.079 2.111 2.976 0.78755393E+000 1.00 C

HETATM 1088 C ATT A 144 -0.079 -1.794 2.976 0.78797894E+000 1.00 C

HETATM 1089 C ATT A 144 0.016 -1.857 2.849 0.78815912E+000 1.00 C

HETATM 1090 C ATT A 145 0.206 2.175 2.976 0.78720431E+000 1.00 C

HETATM 1091 C ATT A 145 0.270 2.175 2.976 0.78711146E+000 1.00 C

HETATM 1092 C ATT A 144 -0.492 -1.826 2.849 0.78838691E+000 1.00 C

HETATM 1093 C ATT A 144 -0.206 -1.699 2.913 0.78813735E+000 1.00 C

HETATM 1094 C ATT A 144 -0.302 -1.699 2.913 0.78830639E+000 1.00 C

HETATM 1095 C ATT A 144 -0.143 -1.730 2.945 0.78841402E+000 1.00 C

HETATM 1096 C ATT A 144 -0.048 -1.762 2.881 0.78824518E+000 1.00 C

HETATM 1097 C ATT A 144 -0.397 -1.730 2.881 0.78824094E+000 1.00 C

HETATM 1098 C ATT A 144 -0.238 -1.667 2.786 0.78800886E+000 1.00 C

HETATM 1099 C ATT A 145 0.206 1.699 2.913 0.78813563E+000 1.00 C

HETATM 1100 C ATT A 145 0.302 1.699 2.913 0.78830812E+000 1.00 C

HETATM 1101 C ATT A 145 0.143 1.730 2.945 0.78841341E+000 1.00 C

HETATM 1102 C ATT A 145 0.079 1.794 2.976 0.78796263E+000 1.00 C

HETATM 1103 C ATT A 145 0.238 1.667 2.786 0.78801127E+000 1.00 C

HETATM 1104 C ATT A 145 0.397 1.730 2.881 0.78823092E+000 1.00 C

HETATM 1105 C ATT A 145 -0.016 1.953 2.913 0.78854216E+000 1.00 C

HETATM 1106 C ATT A 145 0.048 1.762 2.881 0.78823898E+000 1.00 C

HETATM 1107 C ATT A 145 0.492 1.826 2.849 0.78838116E+000 1.00 C

HETATM 1108 C ATT A 145 -0.016 1.857 2.849 0.78817883E+000 1.00 C

HETATM 1109 C ATT A 145 0.016 2.080 2.913 0.78839107E+000 1.00 C

HETATM 1110 C ATT A 145 0.492 2.080 2.849 0.78842231E+000 1.00 C

HETATM 1111 C ATT A 145 0.016 1.826 2.913 0.78845094E+000 1.00 C

HETATM 1112 C ATT A 145 0.492 2.048 2.913 0.78801356E+000 1.00 C

HETATM 1113 C ATT A 145 0.143 2.207 2.881 0.78804029E+000 1.00 C

HETATM 1114 C ATT A 145 0.238 2.238 2.786 0.78843037E+000 1.00 C

HETATM 1115 C ATT A 145 0.302 2.207 2.913 0.78755290E+000 1.00 C

HETATM 1116 C ATT A 145 0.524 1.953 2.849 0.78854530E+000 1.00 C

HETATM 1117 C ATT A 149 0.238 1.953 2.881 0.77236821E+000 1.00 C

HETATM 1118 C ATT A 145 0.492 1.889 2.913 0.78824242E+000 1.00 C

HETATM 1119 C ATT A 145 -0.048 1.953 2.786 0.78735094E+000 1.00 C

HETATM 1120 C ATT A 150 0.238 1.953 2.786 0.96009858E+000 1.00 C

HETATM 1121 C ATT A 149 0.302 1.953 2.849 0.77562447E+000 1.00 C

HETATM 1122 C ATT A 145 -0.016 2.048 2.849 0.78830367E+000 1.00 C

HETATM 1123 C ATT A 149 0.238 2.016 2.849 0.77536092E+000 1.00 C

HETATM 1124 C ATT A 145 0.111 2.207 2.786 0.78847337E+000 1.00 C

HETATM 1125 C ATT A 145 0.365 2.207 2.849 0.78815976E+000 1.00 C

HETATM 1126 C ATT A 145 0.016 2.111 2.849 0.78837003E+000 1.00 C

HETATM 1127 C ATT A 145 0.460 2.143 2.786 0.78832423E+000 1.00 C

HETATM 1128 C ATT A 145 0.079 2.175 2.722 0.78848610E+000 1.00 C

HETATM 1129 C ATT A 146 -0.175 -1.984 2.818 0.77617339E+000 1.00 C

HETATM 1130 C ATT A 144 -0.460 -1.762 2.786 0.78776049E+000 1.00 C

HETATM 1131 C ATT A 144 -0.302 -2.207 2.691 0.78833209E+000 1.00 C

HETATM 1132 C ATT A 144 -0.365 -2.207 2.754 0.78853786E+000 1.00 C

HETATM 1133 C ATT A 144 -0.175 -2.207 2.691 0.78852817E+000 1.00 C

HETATM 1134 C ATT A 144 -0.079 -2.175 2.722 0.78849503E+000 1.00 C

HETATM 1135 C ATT A 144 -0.429 -2.143 2.691 0.78846484E+000 1.00 C

HETATM 1136 C ATT A 144 0.016 -2.048 2.722 0.78827461E+000 1.00 C

HETATM 1137 C ATT A 144 -0.492 -2.080 2.754 0.78841851E+000 1.00 C

HETATM 1138 C ATT A 144 -0.302 -2.175 2.627 0.78835637E+000 1.00 C

HETATM 1139 C ATT A 144 -0.206 -2.175 2.627 0.78828678E+000 1.00 C

HETATM 1140 C ATT A 144 -0.079 -2.143 2.659 0.78823964E+000 1.00 C

HETATM 1141 C ATT A 144 -0.492 -2.048 2.691 0.78828097E+000 1.00 C

HETATM 1142 C ATT A 144 -0.365 -2.143 2.627 0.78829845E+000 1.00 C

HETATM 1143 C ATT A 144 -0.524 -1.984 2.754 0.78841806E+000 1.00 C

HETATM 1144 C ATT A 144 -0.492 -1.953 2.659 0.78814636E+000 1.00 C

HETATM 1145 C ATT A 144 -0.143 -2.080 2.564 0.78809397E+000 1.00 C

HETATM 1146 C ATT A 144 -0.397 -2.016 2.564 0.78797107E+000 1.00 C

HETATM 1147 C ATT A 144 -0.270 -2.048 2.532 0.78806333E+000 1.00 C

HETATM 1148 C ATT A 144 -0.206 -2.048 2.532 0.78808130E+000 1.00 C

HETATM 1149 C ATT A 144 0.016 -1.984 2.691 0.78810181E+000 1.00 C

HETATM 1150 C ATT A 144 -0.238 -1.953 2.500 0.78515537E+000 1.00 C

HETATM 1151 C ATT A 144 -0.397 -1.889 2.564 0.78806930E+000 1.00 C

HETATM 1152 C ATT A 146 -0.238 -1.953 2.722 0.77561657E+000 1.00 C

HETATM 1153 C ATT A 144 -0.048 -1.921 2.595 0.78811347E+000 1.00 C

HETATM 1154 C ATT A 144 -0.333 -1.921 2.532 0.78817548E+000 1.00 C

HETATM 1155 C ATT A 144 -0.460 -1.889 2.627 0.78804106E+000 1.00 C

HETATM 1156 C ATT A 144 0.016 -1.921 2.691 0.78803615E+000 1.00 C

HETATM 1157 C ATT A 145 0.460 1.762 2.786 0.78778852E+000 1.00 C

HETATM 1158 C ATT A 144 -0.492 -1.857 2.691 0.78798305E+000 1.00 C

HETATM 1159 C ATT A 144 -0.365 -1.794 2.595 0.78832817E+000 1.00 C

HETATM 1160 C ATT A 144 -0.270 -1.794 2.564 0.78856964E+000 1.00 C

HETATM 1161 C ATT A 144 -0.206 -1.857 2.532 0.78852320E+000 1.00 C

HETATM 1162 C ATT A 144 -0.143 -1.826 2.564 0.78848478E+000 1.00 C

HETATM 1163 C ATT A 144 -0.016 -1.857 2.659 0.78807250E+000 1.00 C

HETATM 1164 C ATT A 144 -0.206 -1.794 2.564 0.78857639E+000 1.00 C

HETATM 1165 C ATT A 144 -0.079 -1.794 2.627 0.78826512E+000 1.00 C

HETATM 1166 C ATT A 144 0.016 -1.857 2.722 0.78799194E+000 1.00 C

HETATM 1167 C ATT A 144 -0.429 -1.762 2.691 0.78801187E+000 1.00 C

HETATM 1168 C ATT A 144 -0.302 -1.699 2.691 0.78809868E+000 1.00 C

HETATM 1169 C ATT A 149 0.175 1.984 2.818 0.77617494E+000 1.00 C

HETATM 1170 C ATT A 144 -0.048 -1.762 2.722 0.78807956E+000 1.00 C

HETATM 1171 C ATT A 144 -0.492 -1.826 2.754 0.78809369E+000 1.00 C

HETATM 1172 C ATT A 144 -0.175 -1.699 2.691 0.78824777E+000 1.00 C

HETATM 1173 C ATT A 144 -0.365 -1.699 2.754 0.78806771E+000 1.00 C

HETATM 1174 C ATT A 146 -0.175 -1.921 2.786 0.77616382E+000 1.00 C

HETATM 1175 C ATT A 146 -0.238 -1.889 2.754 0.77544200E+000 1.00 C

HETATM 1176 C ATT A 145 0.048 1.762 2.722 0.78808212E+000 1.00 C

HETATM 1177 C ATT A 149 0.238 1.889 2.754 0.77544550E+000 1.00 C

HETATM 1178 C ATT A 149 0.175 1.921 2.786 0.77616933E+000 1.00 C

HETATM 1179 C ATT A 145 0.175 1.699 2.691 0.78824767E+000 1.00 C

HETATM 1180 C ATT A 145 0.302 1.699 2.691 0.78809229E+000 1.00 C

HETATM 1181 C ATT A 145 0.365 1.699 2.754 0.78807057E+000 1.00 C

HETATM 1182 C ATT A 145 0.429 1.762 2.691 0.78802260E+000 1.00 C

HETATM 1183 C ATT A 145 0.492 1.826 2.754 0.78807907E+000 1.00 C

HETATM 1184 C ATT A 145 0.492 1.857 2.691 0.78799866E+000 1.00 C

HETATM 1185 C ATT A 145 0.016 1.857 2.659 0.78807798E+000 1.00 C

HETATM 1186 C ATT A 145 0.079 1.794 2.627 0.78826122E+000 1.00 C

HETATM 1187 C ATT A 145 0.365 1.794 2.595 0.78832885E+000 1.00 C

HETATM 1188 C ATT A 145 0.206 1.794 2.564 0.78857541E+000 1.00 C

HETATM 1189 C ATT A 145 0.270 1.794 2.564 0.78856953E+000 1.00 C

HETATM 1190 C ATT A 145 0.492 1.953 2.659 0.78814678E+000 1.00 C

HETATM 1191 C ATT A 146 -0.302 -1.984 2.754 0.77569735E+000 1.00 C

HETATM 1192 C ATT A 145 -0.016 1.921 2.691 0.78804825E+000 1.00 C

HETATM 1193 C ATT A 145 0.143 1.826 2.564 0.78848298E+000 1.00 C

HETATM 1194 C ATT A 145 0.048 1.921 2.595 0.78811752E+000 1.00 C

HETATM 1195 C ATT A 145 0.206 1.857 2.532 0.78852230E+000 1.00 C

HETATM 1196 C ATT A 145 0.397 1.889 2.564 0.78807844E+000 1.00 C

HETATM 1197 C ATT A 145 0.524 1.984 2.754 0.78842249E+000 1.00 C

HETATM 1198 C ATT A 145 0.238 1.953 2.500 0.78514567E+000 1.00 C

HETATM 1199 C ATT A 149 0.238 1.953 2.722 0.77563103E+000 1.00 C

HETATM 1200 C ATT A 145 -0.016 1.984 2.691 0.78811511E+000 1.00 C

HETATM 1201 C ATT A 145 0.333 1.921 2.532 0.78817167E+000 1.00 C

HETATM 1202 C ATT A 144 -0.111 -1.699 2.786 0.78794833E+000 1.00 C

HETATM 1203 C ATT A 145 0.397 2.016 2.564 0.78797822E+000 1.00 C

HETATM 1204 C ATT A 145 -0.016 2.048 2.722 0.78825942E+000 1.00 C

HETATM 1205 C ATT A 145 0.143 2.080 2.564 0.78809305E+000 1.00 C

HETATM 1206 C ATT A 145 0.206 2.048 2.532 0.78808059E+000 1.00 C

HETATM 1207 C ATT A 145 0.270 2.048 2.532 0.78806373E+000 1.00 C

HETATM 1208 C ATT A 145 0.492 2.048 2.691 0.78829300E+000 1.00 C

HETATM 1209 C ATT A 145 0.079 2.111 2.627 0.78823161E+000 1.00 C

HETATM 1210 C ATT A 145 0.206 2.175 2.627 0.78829217E+000 1.00 C

HETATM 1211 C ATT A 145 0.302 2.175 2.627 0.78835636E+000 1.00 C

HETATM 1212 C ATT A 145 0.365 2.143 2.627 0.78829541E+000 1.00 C

HETATM 1213 C ATT A 145 0.429 2.143 2.691 0.78846985E+000 1.00 C

HETATM 1214 C ATT A 145 0.492 2.080 2.754 0.78840315E+000 1.00 C

HETATM 1215 C ATT A 145 0.175 2.207 2.691 0.78853081E+000 1.00 C

HETATM 1216 C ATT A 145 0.302 2.207 2.691 0.78833220E+000 1.00 C

HETATM 1217 C ATT A 145 0.365 2.207 2.754 0.78853690E+000 1.00 C

HETATM 1218 C ATT A 145 0.111 1.699 2.786 0.78794279E+000 1.00 C

HETATM 1219 C ATT A 149 0.302 1.921 2.754 0.77483864E+000 1.00 C

HETATM 1220 C ATT A 149 0.302 1.984 2.754 0.77577440E+000 1.00 C

HETATM 1221 C ATT A 146 -0.238 -2.016 2.754 0.77600694E+000 1.00 C

HETATM 1222 C ATT A 146 -0.302 -1.921 2.754 0.77468066E+000 1.00 C

HETATM 1223 C ATT A 149 0.238 2.016 2.754 0.77602932E+000 1.00 C

HETATM 1224 C ATT A 144 -0.333 -1.984 2.532 0.78804032E+000 1.00 C

HETATM 1225 C ATT A 144 -0.270 -1.857 2.532 0.78849344E+000 1.00 C

HETATM 1226 C ATT A 145 0.270 1.857 2.532 0.78849304E+000 1.00 C

HETATM 1227 C ATT A 145 0.333 1.984 2.532 0.78803698E+000 1.00 C

The following information is printed according to order of basin labels Basin indices, populations (e), volumes (Å^3) and assigned labels

1 Basin 139 Pop.: 2.0763 Vol.: 0.250 Label: C(B6)

2 Basin 150 Pop.: 3.9894 Vol.: 0.003 Label: C(Br19)

3 Basin 149 Pop.: 6.8830 Vol.: 0.012 Label: C(Br19)

4 Basin 145 Pop.: 16.8734 Vol.: 0.791 Label: C(Br19)

5 Basin 143 Pop.: 4.4816 Vol.: 0.003 Label: C(Br20)

6 Basin 142 Pop.: 3.9182 Vol.: 0.007 Label: C(Br20)

7 Basin 141 Pop.: 4.4427 Vol.: 0.008 Label: C(Br18)

8 Basin 140 Pop.: 4.4854 Vol.: 0.003 Label: C(Br18)

9 Basin 138 Pop.: 2.0763 Vol.: 0.250 Label: C(B3)

10 Basin 135 Pop.: 6.2326 Vol.: 0.003 Label: C(Br14)

11 Basin 137 Pop.: 2.6056 Vol.: 0.004 Label: C(Br20)

12 Basin 136 Pop.: 2.0631 Vol.: 0.003 Label: C(Br18)

13 Basin 148 Pop.: 4.2136 Vol.: 0.003 Label: C(Br22)

14 Basin 147 Pop.: 1.5874 Vol.: 0.002 Label: C(Br22)

15 Basin 146 Pop.: 5.0874 Vol.: 0.009 Label: C(Br22)

16 Basin 133 Pop.: 0.8818 Vol.: 0.002 Label: C(Br14)

17 Basin 144 Pop.: 16.8679 Vol.: 0.792 Label: C(Br22)

18 Basin 132 Pop.: 5.0032 Vol.: 0.009 Label: C(Br14)

19 Basin 129 Pop.: 2.0771 Vol.: 0.249 Label: C(B1)

20 Basin 128 Pop.: 2.0770 Vol.: 0.249 Label: C(B2)

21 Basin 127 Pop.: 5.0541 Vol.: 0.004 Label: C(Br15)

22 Basin 125 Pop.: 5.7445 Vol.: 0.011 Label: C(Br15)

23 Basin 126 Pop.: 5.0496 Vol.: 0.004 Label: C(Br17)

24 Basin 121 Pop.: 5.1358 Vol.: 0.009 Label: C(Br16)

25 Basin 124 Pop.: 5.7393 Vol.: 0.011 Label: C(Br17)

26 Basin 123 Pop.: 16.8807 Vol.: 0.792 Label: C(Br20)

27 Basin 134 Pop.: 6.3489 Vol.: 0.003 Label: C(Br21)

28 Basin 122 Pop.: 16.8865 Vol.: 0.792 Label: C(Br18)

29 Basin 120 Pop.: 6.6386 Vol.: 0.005 Label: C(Br16)

30 Basin 131 Pop.: 4.9040 Vol.: 0.009 Label: C(Br21)

31 Basin 130 Pop.: 0.8624 Vol.: 0.002 Label: C(Br21)

32 Basin 119 Pop.: 6.2640 Vol.: 0.004 Label: C(Br13)

33 Basin 118 Pop.: 5.4865 Vol.: 0.010 Label: C(Br13)

34 Basin 109 Pop.: 2.0756 Vol.: 0.251 Label: C(B9)

35 Basin 107 Pop.: 2.0757 Vol.: 0.251 Label: C(B12)

36 Basin 105 Pop.: 16.9156 Vol.: 0.792 Label: C(Br16)

37 Basin 104 Pop.: 16.9214 Vol.: 0.792 Label: C(Br13)

38 Basin 93 Pop.: 2.0755 Vol.: 0.251 Label: C(B10)

39 Basin 92 Pop.: 2.0753 Vol.: 0.251 Label: C(B8)

40 Basin 63 Pop.: 16.8783 Vol.: 0.790 Label: C(Br15)

41 Basin 57 Pop.: 16.9050 Vol.: 0.791 Label: C(Br14)

42 Basin 53 Pop.: 2.0750 Vol.: 0.249 Label: C(B5)

43 Basin 52 Pop.: 2.0759 Vol.: 0.250 Label: C(B4)

44 Basin 29 Pop.: 2.0757 Vol.: 0.250 Label: C(B11)

45 Basin 26 Pop.: 2.0752 Vol.: 0.250 Label: C(B7)

46 Basin 18 Pop.: 16.8847 Vol.: 0.790 Label: C(Br17)

47 Basin 19 Pop.: 16.8993 Vol.: 0.791 Label: C(Br21)

48 Basin 102 Pop.: 2.1353 Vol.: 0.040 Label: C(O23)

49 Basin 100 Pop.: 2.1364 Vol.: 0.040 Label: C(O26)

50 Basin 74 Pop.: 0.0910 Vol.: 4.557 Label: V(Br16)

51 Basin 78 Pop.: 0.7518 Vol.: 40.463 Label: V(Br18)

52 Basin 76 Pop.: 0.7069 Vol.: 38.111 Label: V(Br18)

53 Basin 70 Pop.: 2.2818 Vol.: 146.693 Label: V(Br16)

54 Basin 67 Pop.: 0.1316 Vol.: 5.999 Label: V(Br13)

55 Basin 66 Pop.: 1.8633 Vol.: 105.354 Label: V(Br13)

56 Basin 64 Pop.: 0.0794 Vol.: 9.054 Label: V(Br14)

57 Basin 10 Pop.: 1.6609 Vol.: 86.483 Label: V(Br17)

58 Basin 62 Pop.: 0.0440 Vol.: 3.564 Label: V(Br15)

59 Basin 61 Pop.: 2.4996 Vol.: 91.394 Label: V(Br15)

60 Basin 60 Pop.: 2.3896 Vol.: 89.674 Label: V(Br13)

61 Basin 59 Pop.: 2.2407 Vol.: 104.485 Label: V(Br14)

62 Basin 58 Pop.: 2.3892 Vol.: 90.947 Label: V(Br16)

63 Basin 77 Pop.: 0.7585 Vol.: 40.783 Label: V(Br20)

64 Basin 56 Pop.: 0.1326 Vol.: 6.097 Label: V(Br16)

65 Basin 55 Pop.: 2.4409 Vol.: 161.781 Label: V(Br15)

66 Basin 51 Pop.: 2.3640 Vol.: 129.712 Label: V(Br14)

67 Basin 36 Pop.: 1.8612 Vol.: 105.772 Label: V(Br16)

68 Basin 117 Pop.: 0.1231 Vol.: 3.840 Label: V(Br14)

69 Basin 65 Pop.: 1.4504 Vol.: 83.210 Label: V(Br20)

70 Basin 31 Pop.: 1.1883 Vol.: 36.109 Label: V(Br18)

71 Basin 16 Pop.: 2.3719 Vol.: 150.580 Label: V(Br13)

72 Basin 17 Pop.: 2.5107 Vol.: 156.977 Label: V(Br18)

73 Basin 15 Pop.: 0.0437 Vol.: 3.553 Label: V(Br17)

74 Basin 14 Pop.: 2.4412 Vol.: 161.606 Label: V(Br17)

75 Basin 13 Pop.: 0.0475 Vol.: 3.220 Label: V(Br17)

76 Basin 12 Pop.: 2.4998 Vol.: 91.349 Label: V(Br17)

77 Basin 88 Pop.: 0.0477 Vol.: 3.713 Label: V(Br15)

78 Basin 86 Pop.: 0.3341 Vol.: 23.324 Label: V(Br14)

79 Basin 5 Pop.: 2.2399 Vol.: 104.478 Label: V(Br21)

80 Basin 85 Pop.: 1.5441 Vol.: 103.275 Label: V(Br14)

81 Basin 48 Pop.: 2.5109 Vol.: 158.308 Label: V(Br20)

82 Basin 83 Pop.: 1.6613 Vol.: 86.445 Label: V(Br15)

83 Basin 91 Pop.: 0.8473 Vol.: 45.946 Label: V(Br19)

84 Basin 4 Pop.: 0.0794 Vol.: 9.267 Label: V(Br21)

85 Basin 3 Pop.: 2.3646 Vol.: 130.947 Label: V(Br21)

86 Basin 73 Pop.: 1.4800 Vol.: 45.764 Label: V(Br22)

87 Basin 72 Pop.: 0.8062 Vol.: 26.692 Label: V(Br22)

88 Basin 71 Pop.: 0.3973 Vol.: 15.842 Label: V(Br22)

89 Basin 24 Pop.: 1.1881 Vol.: 36.517 Label: V(Br20)

90 Basin 69 Pop.: 2.4569 Vol.: 61.427 Label: V(O23)

91 Basin 2 Pop.: 0.3340 Vol.: 23.619 Label: V(Br21)

92 Basin 90 Pop.: 1.2392 Vol.: 93.447 Label: V(Br19)

93 Basin 1 Pop.: 1.5438 Vol.: 103.358 Label: V(Br21)

94 Basin 108 Pop.: 0.1233 Vol.: 3.892 Label: V(Br21)

95 Basin 89 Pop.: 1.8242 Vol.: 108.855 Label: V(Br19)

96 Basin 79 Pop.: 1.4508 Vol.: 82.436 Label: V(Br18)

97 Basin 87 Pop.: 0.3980 Vol.: 15.828 Label: V(Br19)

98 Basin 81 Pop.: 0.8062 Vol.: 26.677 Label: V(Br19)

99 Basin 82 Pop.: 1.4800 Vol.: 45.728 Label: V(Br19)

100 Basin 84 Pop.: 0.7000 Vol.: 38.088 Label: V(Br20)

101 Basin 8 Pop.: 0.8472 Vol.: 45.949 Label: V(Br22)

102 Basin 23 Pop.: 1.2390 Vol.: 93.408 Label: V(Br22)

103 Basin 11 Pop.: 1.8242 Vol.: 108.855 Label: V(Br22)

104 Basin 7 Pop.: 2.4564 Vol.: 61.450 Label: V(O26)

105 Basin 41 Pop.: 0.6606 Vol.: 1.541 Label: V(B8,B9)

106 Basin 47 Pop.: 0.9179 Vol.: 2.155 Label: V(B4,B9)

107 Basin 49 Pop.: 0.6458 Vol.: 1.462 Label: V(B4,B5)

108 Basin 101 Pop.: 0.7341 Vol.: 1.746 Label: V(B2,B3)

109 Basin 103 Pop.: 0.7336 Vol.: 1.745 Label: V(B1,B6)

110 Basin 22 Pop.: 0.6463 Vol.: 1.463 Label: V(B7,B11)

111 Basin 34 Pop.: 0.9031 Vol.: 2.184 Label: V(B3,B8)

112 Basin 44 Pop.: 0.6931 Vol.: 1.606 Label: V(B9,B10)

113 Basin 112 Pop.: 0.8930 Vol.: 1.963 Label: V(B2,B11)

114 Basin 113 Pop.: 0.6813 Vol.: 1.558 Label: V(B6,B11)

115 Basin 50 Pop.: 1.4615 Vol.: 3.158 Label: V(B4,Br14)

116 Basin 39 Pop.: 0.6604 Vol.: 1.540 Label: V(B10,B12)

117 Basin 20 Pop.: 1.4316 Vol.: 3.109 Label: V(B7,Br17)

118 Basin 54 Pop.: 1.4315 Vol.: 3.109 Label: V(B5,Br15)

119 Basin 27 Pop.: 0.9182 Vol.: 2.156 Label: V(B11,B12)

120 Basin 21 Pop.: 1.4614 Vol.: 3.158 Label: V(B11,Br21)

121 Basin 98 Pop.: 1.3919 Vol.: 3.025 Label: V(B3,Br13)

122 Basin 99 Pop.: 1.3923 Vol.: 3.025 Label: V(B6,Br16)

123 Basin 30 Pop.: 1.5320 Vol.: 3.316 Label: V(B8,Br18)

124 Basin 116 Pop.: 0.8931 Vol.: 1.964 Label: V(B1,B4)

125 Basin 114 Pop.: 0.6809 Vol.: 1.557 Label: V(B3,B4)

126 Basin 95 Pop.: 1.7890 Vol.: 2.072 Label: V(B1,O23)

127 Basin 37 Pop.: 0.9031 Vol.: 2.183 Label: V(B6,B10)

128 Basin 38 Pop.: 0.6932 Vol.: 1.607 Label: V(B8,B12)

129 Basin 110 Pop.: 1.5435 Vol.: 3.328 Label: V(B9,Br19)

130 Basin 106 Pop.: 1.5438 Vol.: 3.328 Label: V(B12,Br22)

131 Basin 35 Pop.: 1.5321 Vol.: 3.316 Label: V(B10,Br20)

132 Basin 94 Pop.: 1.7876 Vol.: 2.072 Label: V(B2,O26)

133 Basin 80 Pop.: 1.8286 Vol.: 48.086 Label: V(O23,H24)

134 Basin 75 Pop.: 1.8336 Vol.: 74.994 Label: V(O23,H25)

135 Basin 6 Pop.: 1.8345 Vol.: 75.060 Label: V(O26,H27)

136 Basin 9 Pop.: 1.8286 Vol.: 47.986 Label: V(O26,H28)

137 Basin 97 Pop.: 0.9725 Vol.: 2.250 Label: V(B1,B3,B4)

138 Basin 33 Pop.: 0.7209 Vol.: 1.704 Label: V(B3,B7,B8)

139 Basin 46 Pop.: 0.9045 Vol.: 2.176 Label: V(B4,B5,B9)

140 Basin 45 Pop.: 0.7209 Vol.: 1.704 Label: V(B5,B6,B10)

141 Basin 96 Pop.: 0.9723 Vol.: 2.251 Label: V(B2,B6,B11)

142 Basin 42 Pop.: 0.9671 Vol.: 2.298 Label: V(B4,B8,B9)

143 Basin 28 Pop.: 1.0048 Vol.: 2.434 Label: V(B7,B8,B12)

144 Basin 43 Pop.: 1.0044 Vol.: 2.433 Label: V(B5,B9,B10)

145 Basin 25 Pop.: 0.9037 Vol.: 2.174 Label: V(B7,B11,B12)

146 Basin 32 Pop.: 0.9671 Vol.: 2.297 Label: V(B10,B11,B12)

147 Basin 68 Pop.: 1.5304 Vol.: 4.336 Label: V(B1,B2,B3,B6)

148 Basin 115 Pop.: 1.2889 Vol.: 2.822 Label: V(B1,B4,B5,B6)

149 Basin 111 Pop.: 1.2884 Vol.: 2.822 Label: V(B2,B3,B7,B11)

150 Basin 40 Pop.: 1.0984 Vol.: 2.670 Label: V(B8,B9,B10,B12)

Number of core basins is 49, their indices:

18,19,26,29,52,53,57,63,92,93,100,102,104,105,107,109,118-150

Number of 1-synaptic basins is 55, their indices:

1-5,7,8,10-17,23,24,31,36,48,51,55,56,58-62,64-67,69-74,76-79,81-91,108,117

Number of 2-synaptic basins is 32, their indices:

6,9,20-22,27,30,34,35,37-39,41,44,47,49,50,54,75,80,94,95,98,99,101,103,106,110,112-114,116

Number of 3-synaptic basins is 10, their indices:

25,28,32,33,42,43,45,46,96,97

Number of 4-synaptic basins is 4, their indices:

40,68,111,115

SV.2   Output for $[B_{12}I_{10}(H_2O)_2]^{-\bullet}$

HETATM 1 C ATT A 1 -4.747 -5.699 1.263 0.15797241E-003 1.00 C

HETATM 2 C ATT A 2 -3.223 -2.778 -0.769 0.92519149E+000 1.00 C

HETATM 3 C ATT A 3 -1.667 -3.985 -0.230 0.92495769E+000 1.00 C

HETATM 4 C ATT A 4 -1.032 -2.683 2.818 0.92208228E+000 1.00 C

HETATM 5 C ATT A 5 -0.524 -3.032 2.596 0.92162752E+000 1.00 C

HETATM 6 C ATT A 6 1.032 -4.175 -0.357 0.92324581E+000 1.00 C

HETATM 7 C ATT A 5 -0.429 -3.064 2.596 0.92157212E+000 1.00 C

HETATM 8 C ATT A 5 -0.302 -3.096 2.596 0.92148919E+000 1.00 C

HETATM 9 C ATT A 5 -0.175 -3.096 2.564 0.92149488E+000 1.00 C

HETATM 10 C ATT A 5 0.016 -3.096 2.596 0.92154701E+000 1.00 C

HETATM 11 C ATT A 7 0.175 -3.921 -3.627 0.92320702E+000 1.00 C

HETATM 12 C ATT A 6 1.064 -4.175 -0.293 0.92325679E+000 1.00 C

HETATM 13 C ATT A 8 3.889 -6.144 1.358 0.23805083E-003 1.00 C

HETATM 14 C ATT A 5 0.175 -3.064 2.628 0.92163539E+000 1.00 C

HETATM 15 C ATT A 5 0.333 -3.000 2.660 0.92176770E+000 1.00 C

HETATM 16 C ATT A 9 2.715 -3.254 -0.992 0.92367194E+000 1.00 C

HETATM 17 C ATT A 10 3.508 -1.159 -2.611 0.91722894E+000 1.00 C

HETATM 18 C ATT A 10 3.445 -1.191 -2.674 0.91720650E+000 1.00 C

HETATM 19 C ATT A 11 0.714 -2.715 2.882 0.92201300E+000 1.00 C

HETATM 20 C ATT A 12 2.207 -3.699 0.278 0.91184114E+000 1.00 C

HETATM 21 C ATT A 9 2.746 -3.254 -0.928 0.92368129E+000 1.00 C

HETATM 22 C ATT A 13 3.921 -0.937 1.040 0.92181591E+000 1.00 C

HETATM 23 C ATT A 13 3.953 -0.873 1.009 0.92182612E+000 1.00 C

HETATM 24 C ATT A 14 6.969 -1.413 -3.024 0.13425569E-003 1.00 C

HETATM 25 C ATT A 13 3.985 -0.810 0.977 0.92183079E+000 1.00 C

HETATM 26 C ATT A 15 3.858 -1.064 1.136 0.92179601E+000 1.00 C

HETATM 27 C ATT A 13 4.016 -0.683 0.913 0.92183893E+000 1.00 C

HETATM 28 C ATT A 16 -3.699 -0.683 -2.452 0.91840778E+000 1.00 C

HETATM 29 C ATT A 17 -4.048 -0.238 1.009 0.92183005E+000 1.00 C

HETATM 30 C ATT A 18 -1.508 -2.080 -0.388 0.88567819E+000 1.00 C

HETATM 31 C ATT A 19 1.159 -2.302 -0.420 0.87943306E+000 1.00 C

HETATM 32 C ATT A 20 -0.111 -1.540 -0.293 0.84527448E+000 1.00 C

HETATM 33 C ATT A 21 -4.016 -0.333 1.072 0.92179311E+000 1.00 C

HETATM 34 C ATT A 13 4.048 -0.619 0.913 0.92182779E+000 1.00 C

HETATM 35 C ATT A 17 -4.080 -0.079 0.945 0.92184033E+000 1.00 C

HETATM 36 C ATT A 22 -6.969 1.413 -3.024 0.13488827E-003 1.00 C

HETATM 37 C ATT A 13 4.048 -0.556 0.882 0.92185283E+000 1.00 C

HETATM 38 C ATT A 23 0.778 -1.476 -0.325 0.99999920E+000 1.00 C

HETATM 39 C ATT A 24 -1.000 -1.349 -0.325 0.99999947E+000 1.00 C

HETATM 40 C ATT A 25 1.191 -0.905 0.183 0.85904644E+000 1.00 C

HETATM 41 C ATT A 13 3.762 -1.191 1.294 0.92181579E+000 1.00 C

HETATM 42 C ATT A 26 -1.540 -2.651 -4.389 0.85154554E+000 1.00 C

HETATM 43 C ATT A 21 -3.985 -0.429 1.136 0.92179274E+000 1.00 C

HETATM 44 C ATT A 27 2.175 -0.175 1.009 0.91240631E+000 1.00 C

HETATM 45 C ATT A 13 4.080 -0.429 0.882 0.92183917E+000 1.00 C

HETATM 46 C ATT A 28 -1.318 -0.714 0.183 0.85722488E+000 1.00 C

HETATM 47 C ATT A 17 -4.080 -0.016 0.913 0.92185776E+000 1.00 C

HETATM 48 C ATT A 29 0.460 -1.286 0.469 0.84836058E+000 1.00 C

HETATM 49 C ATT A 30 -0.619 -1.222 0.469 0.85109917E+000 1.00 C

HETATM 50 C ATT A 31 1.222 -0.841 -0.833 0.84343036E+000 1.00 C

HETATM 51 C ATT A 17 -4.080 0.111 0.882 0.92185258E+000 1.00 C

HETATM 52 C ATT A 32 -2.175 0.175 1.009 0.91241514E+000 1.00 C

HETATM 53 C ATT A 33 3.985 -0.397 -2.071 0.91507856E+000 1.00 C

HETATM 54 C ATT A 34 1.603 -0.111 -0.388 0.84528689E+000 1.00 C

HETATM 55 C ATT A 35 -1.381 -0.651 -0.769 0.84733579E+000 1.00 C

HETATM 56 C ATT A 13 4.080 -0.302 0.850 0.92183883E+000 1.00 C

HETATM 57 C ATT A 36 -1.603 0.111 -0.388 0.84527415E+000 1.00 C

HETATM 58 C ATT A 17 -4.080 0.302 0.850 0.92183381E+000 1.00 C

HETATM 59 C ATT A 37 3.699 0.683 -2.452 0.91841051E+000 1.00 C

HETATM 60 C ATT A 38 -0.810 -0.397 0.945 0.84117587E+000 1.00 C

HETATM 61 C ATT A 39 -0.016 0.016 1.231 0.85455084E+000 1.00 C

HETATM 62 C ATT A 40 0.746 -0.524 0.945 0.84195575E+000 1.00 C

HETATM 63 C ATT A 41 0.810 0.397 0.945 0.84122961E+000 1.00 C

HETATM 64 C ATT A 42 1.318 0.714 0.183 0.85713686E+000 1.00 C

HETATM 65 C ATT A 43 1.381 0.651 -0.769 0.84733537E+000 1.00 C

HETATM 66 C ATT A 13 4.080 -0.079 0.882 0.92184987E+000 1.00 C

HETATM 67 C ATT A 44 -1.254 0.841 -0.801 0.84345127E+000 1.00 C

HETATM 68 C ATT A 45 -1.191 0.905 0.183 0.85893508E+000 1.00 C

HETATM 69 C ATT A 46 -0.746 0.524 0.945 0.84202336E+000 1.00 C

HETATM 70 C ATT A 13 3.508 -1.318 1.707 0.92188855E+000 1.00 C

HETATM 71 C ATT A 13 4.080 0.016 0.913 0.92185384E+000 1.00 C

HETATM 72 C ATT A 47 -0.429 1.318 0.437 0.84843325E+000 1.00 C

HETATM 73 C ATT A 48 0.651 1.222 0.469 0.85105893E+000 1.00 C

HETATM 74 C ATT A 49 0.111 1.540 -0.293 0.84529593E+000 1.00 C

HETATM 75 C ATT A 50 -3.985 0.397 -2.071 0.91507997E+000 1.00 C

HETATM 76 C ATT A 13 4.080 0.111 0.945 0.92183815E+000 1.00 C

HETATM 77 C ATT A 17 -4.080 0.429 0.882 0.92184366E+000 1.00 C

HETATM 78 C ATT A 17 -4.048 0.556 0.882 0.92185054E+000 1.00 C

HETATM 79 C ATT A 13 4.048 0.238 1.009 0.92182437E+000 1.00 C

HETATM 80 C ATT A 17 -4.048 0.619 0.913 0.92182919E+000 1.00 C

HETATM 81 C ATT A 51 -3.508 1.159 -2.611 0.91722721E+000 1.00 C

HETATM 82 C ATT A 17 -4.016 0.683 0.913 0.92183578E+000 1.00 C

HETATM 83 C ATT A 17 -3.985 0.810 0.977 0.92182973E+000 1.00 C

HETATM 84 C ATT A 52 4.016 0.365 1.072 0.92178527E+000 1.00 C

HETATM 85 C ATT A 17 -3.953 0.873 1.009 0.92182493E+000 1.00 C

HETATM 86 C ATT A 52 3.985 0.429 1.136 0.92178775E+000 1.00 C

HETATM 87 C ATT A 53 1.000 1.349 -0.325 0.99999944E+000 1.00 C

HETATM 88 C ATT A 54 -3.921 0.937 1.040 0.92181303E+000 1.00 C

HETATM 89 C ATT A 55 1.508 2.080 -0.388 0.88572085E+000 1.00 C

HETATM 90 C ATT A 56 3.223 2.778 -0.769 0.92520356E+000 1.00 C

HETATM 91 C ATT A 57 -0.778 1.476 -0.325 0.99999919E+000 1.00 C

HETATM 92 C ATT A 54 -3.858 1.064 1.136 0.92179205E+000 1.00 C

HETATM 93 C ATT A 58 -1.159 2.302 -0.420 0.87936020E+000 1.00 C

HETATM 94 C ATT A 54 -3.762 1.191 1.294 0.92181311E+000 1.00 C

HETATM 95 C ATT A 59 -2.746 3.254 -0.928 0.92368109E+000 1.00 C

HETATM 96 C ATT A 13 3.635 -1.286 1.517 0.92186159E+000 1.00 C

HETATM 97 C ATT A 60 1.667 3.985 -0.230 0.92496157E+000 1.00 C

HETATM 98 C ATT A 61 -2.207 3.699 0.278 0.91183770E+000 1.00 C

HETATM 99 C ATT A 62 -1.064 4.175 -0.293 0.92325076E+000 1.00 C

HETATM 100 C ATT A 4 -1.095 -2.588 2.882 0.92210106E+000 1.00 C

HETATM 101 C ATT A 62 -1.032 4.175 -0.357 0.92324068E+000 1.00 C

HETATM 102 C ATT A 13 3.477 -1.318 1.771 0.92188995E+000 1.00 C

HETATM 103 C ATT A 11 0.778 -2.619 2.945 0.92201168E+000 1.00 C

HETATM 104 C ATT A 63 4.747 5.699 1.263 0.15828907E-003 1.00 C

HETATM 105 C ATT A 4 -1.127 -2.524 2.914 0.92210522E+000 1.00 C

HETATM 106 C ATT A 17 -3.667 -0.746 1.739 0.92182055E+000 1.00 C

HETATM 107 C ATT A 11 0.810 -2.556 2.977 0.92200095E+000 1.00 C

HETATM 108 C ATT A 13 3.381 -1.286 1.929 0.92186856E+000 1.00 C

HETATM 109 C ATT A 64 -3.921 6.144 1.326 0.23771928E-003 1.00 C

HETATM 110 C ATT A 4 -1.159 -2.429 2.977 0.92207829E+000 1.00 C

HETATM 111 C ATT A 13 3.667 -1.254 1.453 0.92183842E+000 1.00 C

HETATM 112 C ATT A 13 3.350 -1.254 2.025 0.92184517E+000 1.00 C

HETATM 113 C ATT A 11 0.841 -2.461 3.041 0.92195820E+000 1.00 C

HETATM 114 C ATT A 17 -3.635 -0.746 1.802 0.92182237E+000 1.00 C

HETATM 115 C ATT A 51 -3.445 1.191 -2.706 0.91719357E+000 1.00 C

HETATM 116 C ATT A 65 3.318 -1.222 2.088 0.92181070E+000 1.00 C

HETATM 117 C ATT A 65 3.286 -1.191 2.152 0.92178563E+000 1.00 C

HETATM 118 C ATT A 17 -3.604 -0.746 1.866 0.92183001E+000 1.00 C

HETATM 119 C ATT A 65 3.254 -1.159 2.215 0.92175311E+000 1.00 C

HETATM 120 C ATT A 66 -3.508 -0.714 2.025 0.92180563E+000 1.00 C

HETATM 121 C ATT A 11 0.873 -2.365 3.104 0.92191576E+000 1.00 C

HETATM 122 C ATT A 4 -1.191 -2.334 3.041 0.92201117E+000 1.00 C

HETATM 123 C ATT A 66 -3.445 -0.683 2.120 0.92178094E+000 1.00 C

HETATM 124 C ATT A 21 -3.762 -0.714 1.580 0.92179899E+000 1.00 C

HETATM 125 C ATT A 13 3.731 -1.222 1.358 0.92183036E+000 1.00 C

HETATM 126 C ATT A 11 0.873 -2.238 3.199 0.92189553E+000 1.00 C

HETATM 127 C ATT A 66 -3.413 -0.651 2.183 0.92176549E+000 1.00 C

HETATM 128 C ATT A 66 -3.381 -0.619 2.247 0.92174161E+000 1.00 C

HETATM 129 C ATT A 67 0.619 -1.095 -3.341 0.80297647E+000 1.00 C

HETATM 130 C ATT A 68 -0.810 -1.540 3.580 0.92203890E+000 1.00 C

HETATM 131 C ATT A 69 0.492 -1.572 3.612 0.92230589E+000 1.00 C

HETATM 132 C ATT A 11 0.841 -2.048 3.326 0.92192538E+000 1.00 C

HETATM 133 C ATT A 11 0.873 -2.175 3.231 0.92188638E+000 1.00 C

HETATM 134 C ATT A 70 -1.159 -2.016 3.263 0.92185882E+000 1.00 C

HETATM 135 C ATT A 70 -1.127 -1.921 3.326 0.92184896E+000 1.00 C

HETATM 136 C ATT A 70 -1.095 -1.857 3.358 0.92186100E+000 1.00 C

HETATM 137 C ATT A 68 -0.524 -1.413 3.676 0.92215189E+000 1.00 C

HETATM 138 C ATT A 69 0.333 -1.476 3.676 0.92232151E+000 1.00 C

HETATM 139 C ATT A 71 3.159 -0.968 2.406 0.92170221E+000 1.00 C

HETATM 140 C ATT A 68 -0.333 -1.381 3.707 0.92218265E+000 1.00 C

HETATM 141 C ATT A 69 0.048 -1.381 3.707 0.92223216E+000 1.00 C

HETATM 142 C ATT A 69 0.429 -1.540 3.644 0.92232924E+000 1.00 C

HETATM 143 C ATT A 68 -0.619 -1.445 3.644 0.92212494E+000 1.00 C

HETATM 144 C ATT A 69 -0.048 -1.381 3.739 0.92222269E+000 1.00 C

HETATM 145 C ATT A 68 -0.746 -1.508 3.612 0.92207943E+000 1.00 C

HETATM 146 C ATT A 69 0.206 -1.445 3.707 0.92230468E+000 1.00 C

HETATM 147 C ATT A 69 0.143 -1.413 3.707 0.92229627E+000 1.00 C

HETATM 148 C ATT A 72 -0.746 -0.968 -3.341 0.79556626E+000 1.00 C

HETATM 149 C ATT A 73 -0.619 1.095 -3.341 0.80290761E+000 1.00 C

HETATM 150 C ATT A 74 0.746 0.968 -3.341 0.79556510E+000 1.00 C

HETATM 151 C ATT A 75 1.540 2.683 -4.357 0.85109911E+000 1.00 C

HETATM 152 C ATT A 71 3.127 -0.841 2.501 0.92172479E+000 1.00 C

HETATM 153 C ATT A 66 -3.286 -0.492 2.406 0.92168997E+000 1.00 C

HETATM 154 C ATT A 66 -3.223 -0.365 2.501 0.92174268E+000 1.00 C

HETATM 155 C ATT A 71 3.096 -0.778 2.533 0.92177207E+000 1.00 C

HETATM 156 C ATT A 76 -0.175 3.921 -3.627 0.92321519E+000 1.00 C

HETATM 157 C ATT A 21 -3.826 -0.683 1.485 0.92177772E+000 1.00 C

HETATM 158 C ATT A 71 3.096 -0.714 2.564 0.92180326E+000 1.00 C

HETATM 159 C ATT A 66 -3.191 -0.302 2.533 0.92178974E+000 1.00 C

HETATM 160 C ATT A 71 3.064 -0.619 2.596 0.92185970E+000 1.00 C

HETATM 161 C ATT A 17 -3.159 -0.238 2.564 0.92182237E+000 1.00 C

HETATM 162 C ATT A 21 -3.858 -0.651 1.421 0.92177468E+000 1.00 C

HETATM 163 C ATT A 71 3.064 -0.524 2.628 0.92193569E+000 1.00 C

HETATM 164 C ATT A 17 -3.127 -0.143 2.596 0.92187537E+000 1.00 C

HETATM 165 C ATT A 77 3.064 -0.238 2.660 0.92202624E+000 1.00 C

HETATM 166 C ATT A 17 -3.127 -0.079 2.628 0.92192725E+000 1.00 C

HETATM 167 C ATT A 21 -3.889 -0.619 1.358 0.92176996E+000 1.00 C

HETATM 168 C ATT A 17 -3.096 0.079 2.660 0.92200729E+000 1.00 C

HETATM 169 C ATT A 13 3.635 0.746 1.802 0.92181919E+000 1.00 C

HETATM 170 C ATT A 13 3.667 0.746 1.739 0.92181774E+000 1.00 C

HETATM 171 C ATT A 77 3.096 -0.079 2.660 0.92200883E+000 1.00 C

HETATM 172 C ATT A 77 3.127 0.079 2.628 0.92192803E+000 1.00 C

HETATM 173 C ATT A 77 3.127 0.143 2.596 0.92187840E+000 1.00 C

HETATM 174 C ATT A 77 3.159 0.238 2.564 0.92182285E+000 1.00 C

HETATM 175 C ATT A 78 3.381 0.619 2.247 0.92174191E+000 1.00 C

HETATM 176 C ATT A 52 3.889 0.619 1.358 0.92176783E+000 1.00 C

HETATM 177 C ATT A 79 3.191 0.302 2.533 0.92179074E+000 1.00 C

HETATM 178 C ATT A 79 3.223 0.365 2.501 0.92174225E+000 1.00 C

HETATM 179 C ATT A 78 3.445 0.683 2.120 0.92178121E+000 1.00 C

HETATM 180 C ATT A 78 3.508 0.714 2.025 0.92180453E+000 1.00 C

HETATM 181 C ATT A 13 3.604 0.746 1.866 0.92182814E+000 1.00 C

HETATM 182 C ATT A 52 3.826 0.683 1.485 0.92177464E+000 1.00 C

HETATM 183 C ATT A 52 3.953 0.524 1.231 0.92177209E+000 1.00 C

HETATM 184 C ATT A 52 3.762 0.714 1.580 0.92179408E+000 1.00 C

HETATM 185 C ATT A 52 3.858 0.651 1.421 0.92177035E+000 1.00 C

HETATM 186 C ATT A 78 3.413 0.651 2.183 0.92176582E+000 1.00 C

HETATM 187 C ATT A 21 -3.921 -0.556 1.263 0.92177476E+000 1.00 C

HETATM 188 C ATT A 17 -3.064 0.206 2.660 0.92202257E+000 1.00 C

HETATM 189 C ATT A 80 0.619 1.445 3.644 0.92211987E+000 1.00 C

HETATM 190 C ATT A 80 0.746 1.508 3.612 0.92207484E+000 1.00 C

HETATM 191 C ATT A 80 0.524 1.413 3.676 0.92214513E+000 1.00 C

HETATM 192 C ATT A 80 0.333 1.381 3.707 0.92217715E+000 1.00 C

HETATM 193 C ATT A 81 0.048 1.381 3.739 0.92221144E+000 1.00 C

HETATM 194 C ATT A 81 -0.048 1.381 3.707 0.92222385E+000 1.00 C

HETATM 195 C ATT A 81 -0.143 1.413 3.707 0.92228886E+000 1.00 C

HETATM 196 C ATT A 81 -0.302 1.476 3.676 0.92231842E+000 1.00 C

HETATM 197 C ATT A 81 -0.206 1.445 3.707 0.92229971E+000 1.00 C

HETATM 198 C ATT A 81 -0.365 1.508 3.676 0.92230989E+000 1.00 C

HETATM 199 C ATT A 80 0.810 1.540 3.580 0.92203543E+000 1.00 C

HETATM 200 C ATT A 81 -0.492 1.572 3.612 0.92229928E+000 1.00 C

HETATM 201 C ATT A 81 -0.429 1.540 3.644 0.92232407E+000 1.00 C

HETATM 202 C ATT A 59 -2.715 3.254 -0.992 0.92366843E+000 1.00 C

HETATM 203 C ATT A 82 -3.096 0.714 2.564 0.92180013E+000 1.00 C

HETATM 204 C ATT A 82 -3.064 0.524 2.628 0.92193366E+000 1.00 C

HETATM 205 C ATT A 17 -3.635 1.286 1.517 0.92185987E+000 1.00 C

HETATM 206 C ATT A 83 -3.254 1.159 2.215 0.92175625E+000 1.00 C

HETATM 207 C ATT A 82 -3.127 0.905 2.469 0.92170650E+000 1.00 C

HETATM 208 C ATT A 17 -3.508 1.318 1.707 0.92188822E+000 1.00 C

HETATM 209 C ATT A 83 -3.286 1.191 2.152 0.92178331E+000 1.00 C

HETATM 210 C ATT A 82 -3.159 0.968 2.406 0.92169903E+000 1.00 C

HETATM 211 C ATT A 82 -3.127 0.841 2.501 0.92172231E+000 1.00 C

HETATM 212 C ATT A 17 -3.731 1.222 1.358 0.92182805E+000 1.00 C

HETATM 213 C ATT A 17 -3.381 1.286 1.929 0.92186773E+000 1.00 C

HETATM 214 C ATT A 17 -3.350 1.254 2.025 0.92184355E+000 1.00 C

HETATM 215 C ATT A 83 -3.318 1.222 2.088 0.92180695E+000 1.00 C

HETATM 216 C ATT A 17 -3.477 1.318 1.771 0.92189066E+000 1.00 C

HETATM 217 C ATT A 17 -3.667 1.254 1.453 0.92183441E+000 1.00 C

HETATM 218 C ATT A 84 1.095 1.857 3.358 0.92185811E+000 1.00 C

HETATM 219 C ATT A 84 1.127 1.921 3.326 0.92184659E+000 1.00 C

HETATM 220 C ATT A 84 1.159 2.016 3.263 0.92185467E+000 1.00 C

HETATM 221 C ATT A 85 -0.841 2.048 3.326 0.92192262E+000 1.00 C

HETATM 222 C ATT A 86 1.191 2.334 3.041 0.92201291E+000 1.00 C

HETATM 223 C ATT A 85 -0.873 2.175 3.231 0.92188128E+000 1.00 C

HETATM 224 C ATT A 85 -0.873 2.270 3.168 0.92189367E+000 1.00 C

HETATM 225 C ATT A 85 -0.873 2.334 3.136 0.92191000E+000 1.00 C

HETATM 226 C ATT A 85 -0.841 2.461 3.041 0.92195777E+000 1.00 C

HETATM 227 C ATT A 85 -0.810 2.556 2.977 0.92199908E+000 1.00 C

HETATM 228 C ATT A 85 -0.714 2.715 2.882 0.92201228E+000 1.00 C

HETATM 229 C ATT A 86 1.032 2.683 2.818 0.92207782E+000 1.00 C

HETATM 230 C ATT A 86 1.127 2.524 2.914 0.92210302E+000 1.00 C

HETATM 231 C ATT A 85 -0.778 2.619 2.945 0.92201075E+000 1.00 C

HETATM 232 C ATT A 87 -0.333 3.000 2.660 0.92176359E+000 1.00 C

HETATM 233 C ATT A 87 0.429 3.064 2.596 0.92156424E+000 1.00 C

HETATM 234 C ATT A 86 1.159 2.429 2.977 0.92207333E+000 1.00 C

HETATM 235 C ATT A 87 -0.175 3.064 2.628 0.92163106E+000 1.00 C

HETATM 236 C ATT A 87 0.302 3.096 2.596 0.92148240E+000 1.00 C

HETATM 237 C ATT A 86 1.095 2.588 2.882 0.92209731E+000 1.00 C

HETATM 238 C ATT A 87 0.619 3.000 2.628 0.92169469E+000 1.00 C

HETATM 239 C ATT A 87 -0.016 3.096 2.596 0.92154301E+000 1.00 C

HETATM 240 C ATT A 87 0.524 3.032 2.596 0.92162195E+000 1.00 C

HETATM 241 C ATT A 87 0.175 3.096 2.564 0.92149113E+000 1.00 C

HETATM 242 C ATT A 87 0.683 2.969 2.628 0.92173929E+000 1.00 C

HETATM 243 C ATT A 88 1.476 -0.111 0.532 0.99999931E+000 1.00 C

HETATM 244 C ATT A 89 -1.476 0.111 0.532 0.99999929E+000 1.00 C

HETATM 245 C ATT A 90 0.810 -1.984 -2.738 0.82722885E+000 1.00 C

HETATM 246 C ATT A 91 -0.810 1.984 -2.738 0.82731556E+000 1.00 C

HETATM 247 C ATT A 92 -1.095 -1.889 -2.674 0.82989487E+000 1.00 C

HETATM 248 C ATT A 93 1.095 1.889 -2.674 0.83004630E+000 1.00 C

HETATM 249 C ATT A 94 -0.206 -2.429 -2.389 0.82742172E+000 1.00 C

HETATM 250 C ATT A 95 0.206 2.429 -2.389 0.82735688E+000 1.00 C

HETATM 251 C ATT A 96 -0.079 -0.905 1.104 0.99999937E+000 1.00 C

HETATM 252 C ATT A 97 0.079 0.905 1.104 0.99999939E+000 1.00 C

HETATM 253 C ATT A 98 0.111 1.349 1.834 0.91213449E+000 1.00 C

HETATM 254 C ATT A 99 -0.079 -1.191 -2.198 0.94565622E+000 1.00 C

HETATM 255 C ATT A 100 0.079 1.191 -2.198 0.94565350E+000 1.00 C

HETATM 256 C ATT A 101 0.651 -0.429 -1.563 0.81949543E+000 1.00 C

HETATM 257 C ATT A 102 -0.111 -1.349 1.834 0.91215319E+000 1.00 C

HETATM 258 C ATT A 103 2.143 -0.143 -1.785 0.86573508E+000 1.00 C

HETATM 259 C ATT A 104 -2.143 0.143 -1.785 0.86558965E+000 1.00 C

HETATM 260 C ATT A 105 3.350 -0.206 -2.770 0.33364430E-004 1.00 C

HETATM 261 C ATT A 106 -3.350 0.206 -2.770 0.33039623E-004 1.00 C

HETATM 262 C ATT A 107 -0.651 0.429 -1.563 0.81957459E+000 1.00 C

HETATM 263 C ATT A 108 0.746 0.397 -1.531 0.80347389E+000 1.00 C

HETATM 264 C ATT A 109 -0.746 -0.397 -1.531 0.80325391E+000 1.00 C

HETATM 265 C ATT A 110 3.032 -0.175 -2.643 0.63974933E-004 1.00 C

HETATM 266 C ATT A 111 -3.032 0.175 -2.643 0.64366479E-004 1.00 C

HETATM 267 C ATT A 112 1.857 -3.635 -0.579 0.17497246E-004 1.00 C

HETATM 268 C ATT A 113 1.667 -3.381 -0.674 0.34322664E-004 1.00 C

HETATM 269 C ATT A 114 0.238 -1.254 -0.992 0.78622763E+000 1.00 C

HETATM 270 C ATT A 114 0.302 -1.222 -1.023 0.78642192E+000 1.00 C

HETATM 271 C ATT A 115 -0.492 -1.159 -1.023 0.79328376E+000 1.00 C

HETATM 272 C ATT A 115 -0.556 -1.127 -1.055 0.79385630E+000 1.00 C

HETATM 273 C ATT A 116 -0.302 1.222 -1.023 0.78628486E+000 1.00 C

HETATM 274 C ATT A 117 0.556 1.127 -1.055 0.79375803E+000 1.00 C

HETATM 275 C ATT A 117 0.492 1.159 -1.023 0.79316865E+000 1.00 C

HETATM 276 C ATT A 116 -0.238 1.254 -0.992 0.78609309E+000 1.00 C

HETATM 277 C ATT A 118 -1.667 3.381 -0.674 0.34323110E-004 1.00 C

HETATM 278 C ATT A 119 -1.857 3.635 -0.579 0.17538020E-004 1.00 C

HETATM 279 C ATT A 120 -2.175 -3.096 -0.611 0.31506837E-004 1.00 C

HETATM 280 C ATT A 121 2.175 3.096 -0.611 0.31622234E-004 1.00 C

HETATM 281 C ATT A 122 -2.397 -3.286 -0.452 0.17104636E-004 1.00 C

HETATM 282 C ATT A 123 2.397 3.286 -0.452 0.17199315E-004 1.00 C

HETATM 283 C ATT A 124 -0.079 -0.841 -1.722 0.99999519E+000 1.00 C

HETATM 284 C ATT A 125 0.079 0.841 -1.722 0.99999516E+000 1.00 C

HETATM 285 C ATT A 126 1.445 -0.111 -1.246 0.99999870E+000 1.00 C

HETATM 286 C ATT A 127 -1.445 0.111 -1.246 0.99999870E+000 1.00 C

HETATM 287 C ATT A 128 -0.143 -2.175 3.104 0.14774002E-004 1.00 C

HETATM 288 C ATT A 129 0.143 2.175 3.104 0.14726165E-004 1.00 C

The following information is printed according to order of basin labels Basin indices, populations (e), volumes ($Å^3$) and assigned labels (Notes: Some basins were marked as "Negligible" since their population is very small. Automatic basin labeling failed in the region of water moieties, therefore the assignment was done manually as discussed in the main text.)

1 Basin 127 Pop.: 2.0777 Vol.: 0.252 Label: C(B3)

2 Basin 125 Pop.: 2.1060 Vol.: 0.208 Label: C(B2)

3 Basin 124 Pop.: 2.1063 Vol.: 0.208 Label: C(B1)

4 Basin 126 Pop.: 2.0778 Vol.: 0.252 Label: C(B6)

5 Basin 24 Pop.: 2.0749 Vol.: 0.250 Label: C(B4)

6 Basin 23 Pop.: 2.0747 Vol.: 0.250 Label: C(B5)

7 Basin 96 Pop.: 2.0733 Vol.: 0.249 Label: C(B9)

8 Basin 89 Pop.: 2.0744 Vol.: 0.249 Label: C(B8)

9 Basin 88 Pop.: 2.0743 Vol.: 0.249 Label: C(B10)

10 Basin 57 Pop.: 2.0747 Vol.: 0.250 Label: C(B7)

11 Basin 53 Pop.: 2.0748 Vol.: 0.250 Label: C(B11)

12 Basin 97 Pop.: 2.0736 Vol.: 0.250 Label: C(B12)

13 Basin 122 Pop.: 10.6699 Vol.: 0.009 Label: C(I14)

14 Basin 120 Pop.: 4.3772 Vol.: 0.004 Label: C(I14)

15 Basin 113 Pop.: 3.2379 Vol.: 0.003 Label: C(I15)

16 Basin 112 Pop.: 11.3864 Vol.: 0.008 Label: C(I15)

17 Basin 111 Pop.: 2.2453 Vol.: 0.001 Label: C(I13)

18 Basin 128 Pop.: 19.4618 Vol.: 0.016 Label: C(I19)

19 Basin 106 Pop.: 11.8891 Vol.: 0.012 Label: C(I13)

20 Basin 105 Pop.: 12.2883 Vol.: 0.012 Label: C(I16)

21 Basin 110 Pop.: 2.2000 Vol.: 0.001 Label: C(I16)

22 Basin 118 Pop.: 3.4352 Vol.: 0.003 Label: C(I17)

23 Basin 119 Pop.: 11.3725 Vol.: 0.009 Label: C(I17)

24 Basin 123 Pop.: 11.0480 Vol.: 0.009 Label: C(I21)

25 Basin 121 Pop.: 4.4112 Vol.: 0.004 Label: C(I21)

26 Basin 129 Pop.: 19.0216 Vol.: 0.016 Label: C(I22)

27 Basin 76 Pop.: 1.7768 Vol.: 291.396 Label: V()

28 Basin 77 Pop.: 8.0403 Vol.: 65.875 Label: V()

29 Basin 78 Pop.: 3.7684 Vol.: 70.257 Label: V()

30 Basin 79 Pop.: 1.9842 Vol.: 26.008 Label: V()

31 Basin 82 Pop.: 4.2742 Vol.: 59.772 Label: V()

32 Basin 83 Pop.: 2.7889 Vol.: 53.936 Label: V()

33 Basin 14 Pop.: 0.0055 Vol.: 118.063 Label: V() Negligible

34 Basin 15 Pop.: 1.0167 Vol.: 10.433 Label: V()

35 Basin 90 Pop.: 1.2522 Vol.: 4.517 Label: V()

36 Basin 91 Pop.: 1.2538 Vol.: 4.519 Label: V()

37 Basin 92 Pop.: 1.3012 Vol.: 4.597 Label: V()

38 Basin 93 Pop.: 1.3035 Vol.: 4.606 Label: V()

39 Basin 94 Pop.: 1.1577 Vol.: 3.663 Label: V()

40 Basin 95 Pop.: 1.1541 Vol.: 3.651 Label: V()

41 Basin 17 Pop.: 28.5613 Vol.: 257.456 Label: V()

42 Basin 21 Pop.: 5.5488 Vol.: 53.412 Label: V()

43 Basin 22 Pop.: 0.0054 Vol.: 119.131 Label: V() Negligible

44 Basin 1 Pop.: 0.0059 Vol.: 312.307 Label: V() Negligible

45 Basin 7 Pop.: 1.7717 Vol.: 290.915 Label: V()

46 Basin 26 Pop.: 1.0948 Vol.: 217.789 Label: V()

47 Basin 52 Pop.: 5.1177 Vol.: 51.322 Label: V()

48 Basin 8 Pop.: 0.0061 Vol.: 284.115 Label: V() Negligible

49 Basin 54 Pop.: 2.7485 Vol.: 29.768 Label: V()

50 Basin 13 Pop.: 22.9545 Vol.: 210.615 Label: V()

51 Basin 63 Pop.: 0.0059 Vol.: 310.676 Label: V() Negligible

52 Basin 64 Pop.: 0.0061 Vol.: 285.198 Label: V() Negligible

53 Basin 65 Pop.: 2.8710 Vol.: 53.991 Label: V()

54 Basin 66 Pop.: 6.0616 Vol.: 98.967 Label: V()

55 Basin 67 Pop.: 1.0266 Vol.: 5.751 Label: V()

56 Basin 71 Pop.: 4.3590 Vol.: 61.014 Label: V()

57 Basin 72 Pop.: 0.9248 Vol.: 4.007 Label: V()

58 Basin 73 Pop.: 1.0275 Vol.: 5.754 Label: V()

59 Basin 74 Pop.: 0.9244 Vol.: 4.013 Label: V()

60 Basin 75 Pop.: 1.0886 Vol.: 217.129 Label: V()

61 Basin 56 Pop.: 16.6557 Vol.: 239.120 Label: V(I21)

62 Basin 6 Pop.: 16.7828 Vol.: 107.965 Label: V(I15)

63 Basin 5 Pop.: 4.7326 Vol.: 107.534 Label: V(I19)

64 Basin 4 Pop.: 6.7683 Vol.: 97.104 Label: V(I19)

65 Basin 51 Pop.: 16.0877 Vol.: 313.739 Label: V(I13)

66 Basin 50 Pop.: 0.2689 Vol.: 1.015 Label: V(I13)

67 Basin 37 Pop.: 14.8027 Vol.: 147.500 Label: V(I16)

68 Basin 33 Pop.: 0.2721 Vol.: 1.009 Label: V(I16)

69 Basin 32 Pop.: 3.3332 Vol.: 3.928 Label: V(B8)

70 Basin 27 Pop.: 3.2554 Vol.: 3.929 Label: V(B10)

71 Basin 12 Pop.: 0.2004 Vol.: 3.553 Label: V(I15)

72 Basin 70 Pop.: 1.3195 Vol.: 24.932 Label: V(I19)

73 Basin 69 Pop.: 7.0199 Vol.: 161.537 Label: V(I19)

74 Basin 68 Pop.: 4.7941 Vol.: 82.178 Label: V(I19)

75 Basin 100 Pop.: 2.1079 Vol.: 1.864 Label: V(B2)

76 Basin 99 Pop.: 2.1088 Vol.: 1.865 Label: V(B1)

77 Basin 11 Pop.: 6.7054 Vol.: 94.358 Label: V(I19)

78 Basin 10 Pop.: 16.0476 Vol.: 311.666 Label: V(I16)

79 Basin 9 Pop.: 16.5516 Vol.: 220.883 Label: V(I15)

80 Basin 3 Pop.: 17.9337 Vol.: 112.520 Label: V(I14)

81 Basin 2 Pop.: 16.3423 Vol.: 239.890 Label: V(I14)

82 Basin 62 Pop.: 16.8228 Vol.: 108.095 Label: V(I17)

83 Basin 61 Pop.: 0.2054 Vol.: 3.502 Label: V(I17)

84 Basin 60 Pop.: 17.3225 Vol.: 112.495 Label: V(I21)

85 Basin 59 Pop.: 16.5379 Vol.: 221.244 Label: V(I17)

86 Basin 16 Pop.: 14.8682 Vol.: 148.504 Label: V(I13)

87 Basin 80 Pop.: 4.7953 Vol.: 81.698 Label: V(I22)

88 Basin 81 Pop.: 6.9915 Vol.: 162.536 Label: V(I22)

89 Basin 86 Pop.: 5.9574 Vol.: 80.611 Label: V(I22)

90 Basin 87 Pop.: 5.5468 Vol.: 123.734 Label: V(I22)

91 Basin 84 Pop.: 1.3178 Vol.: 24.833 Label: V(I22)

92 Basin 85 Pop.: 6.7035 Vol.: 94.348 Label: V(I22)

93 Basin 108 Pop.: 0.5935 Vol.: 1.000 Label: V(B2,B6)

94 Basin 109 Pop.: 0.5921 Vol.: 0.998 Label: V(B1,B3)

95 Basin 114 Pop.: 0.2508 Vol.: 0.388 Label: V(B1,B5)

96 Basin 115 Pop.: 0.3191 Vol.: 0.504 Label: V(B1,B4)

97 Basin 116 Pop.: 0.2497 Vol.: 0.386 Label: V(B2,B7)

98 Basin 36 Pop.: 0.6570 Vol.: 1.571 Label: V(B3,B8)

99 Basin 40 Pop.: 0.6569 Vol.: 1.505 Label: V(B9,B10)

100 Basin 58 Pop.: 5.1892 Vol.: 3.741 Label: V(B7,I17)

101 Basin 117 Pop.: 0.3185 Vol.: 0.503 Label: V(B2,B11)

102 Basin 46 Pop.: 0.6574 Vol.: 1.506 Label: V(B8,B12)

103 Basin 47 Pop.: 0.7185 Vol.: 1.709 Label: V(B7,B12)

104 Basin 30 Pop.: 0.7681 Vol.: 1.803 Label: V(B4,B9)

105 Basin 18 Pop.: 3.5643 Vol.: 3.786 Label: V(B4,I14)

106 Basin 38 Pop.: 0.6426 Vol.: 1.479 Label: V(B8,B9)

107 Basin 19 Pop.: 5.4321 Vol.: 3.742 Label: V(B5,I15)

108 Basin 34 Pop.: 0.6573 Vol.: 1.571 Label: V(B6,B10)

109 Basin 104 Pop.: 7.1660 Vol.: 3.883 Label: V(B3,I13)

110 Basin 29 Pop.: 0.7174 Vol.: 1.706 Label: V(B5,B9)

111 Basin 103 Pop.: 6.9037 Vol.: 3.883 Label: V(B6,I16)

112 Basin 102 Pop.: 3.6626 Vol.: 3.991 Label: V(B9,I19)

113 Basin 41 Pop.: 0.6433 Vol.: 1.480 Label: V(B10,B12)

114 Basin 48 Pop.: 0.7674 Vol.: 1.802 Label: V(B11,B12)

115 Basin 55 Pop.: 3.5142 Vol.: 3.787 Label: V(B11,I21)

116 Basin 98 Pop.: 3.6703 Vol.: 3.990 Label: V(B12,I22)

117 Basin 107 Pop.: 0.9730 Vol.: 1.660 Label: V(B1,B2,B3)

118 Basin 101 Pop.: 1.0929 Vol.: 1.851 Label: V(B1,B2,B6)

119 Basin 28 Pop.: 0.9430 Vol.: 2.209 Label: V(B4,B8,B9)

120 Basin 25 Pop.: 1.0189 Vol.: 2.432 Label: V(B5,B9,B10)

121 Basin 45 Pop.: 1.0173 Vol.: 2.428 Label: V(B7,B8,B12)

122 Basin 42 Pop.: 0.9433 Vol.: 2.209 Label: V(B10,B11,B12)

123 Basin 35 Pop.: 1.4445 Vol.: 3.091 Label: V(B1,B3,B4,B8)

124 Basin 20 Pop.: 1.5201 Vol.: 3.168 Label: V(B1,B4,B5,B9)

125 Basin 31 Pop.: 1.3734 Vol.: 2.946 Label: V(B1,B5,B6,B10)

126 Basin 44 Pop.: 1.3756 Vol.: 2.950 Label: V(B2,B3,B7,B8)

127 Basin 43 Pop.: 1.4444 Vol.: 3.092 Label: V(B2,B6,B10,B11)

128 Basin 49 Pop.: 1.5199 Vol.: 3.168 Label: V(B2,B7,B11,B12)

129 Basin 39 Pop.: 1.0921 Vol.: 2.643 Label: V(B8,B9,B10,B12)

Number of core basins is 26, their indices:

23,24,53,57,88,89,96,97,105,106,110-113,118-129

Number of 1-synaptic basins is 32, their indices:

2-6,9-12,16,27,32,33,37,50,51,56,59-62,68-70,80,81,84-87,99,100

Number of 2-synaptic basins is 24, their indices:

18,19,29,30,34,36,38,40,41,46-48,55,58,98,102-104,108,109,114-117

Number of 3-synaptic basins is 6, their indices:

25,28,42,45,101,107

Number of 4-synaptic basins is 7, their indices:

20,31,35,39,43,44,49