Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

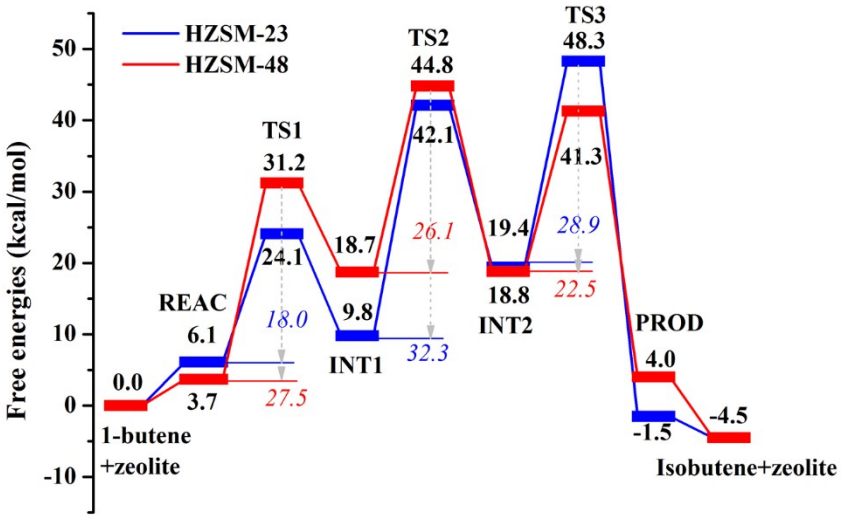

Fig. S1 Free energy profiles of the skeletal isomerization of 1-butene over HZSM-23 and HZSM-48 zeolites at 700 K. The energies in italic are activation energies (E_{an},n=1,2,3), whereas the energies in bold are energy barriers.

Table S1. Comparison of calculated reaction energetics with or without harmonic entropy correction (T=700 K) (kcal/mol)

	without entropy		with entropy	
	HZSM-23	HZSM-48	HZSM-23	HZSM-48
1-butene+zeolite	0.0	0.0	0.0	0.0
Adsorption	-19.0	-19.8	6.1	3.7
TS1	-7.8	0.3	24.1	31.2
INT1	-21.8	-13.8	9.8	18.7
TS2	13.3	18.0	42.1	44.8
INT2	-13.1	-13.9	19.4	18.8
TS3	15.8	11.5	48.3	41.3
Product	-27.8	-21.6	-1.5	4.0
Isobutene+zeolite	-4.2	-4.2	-4.5	-4.5

Appendix:

The coordinates for all stationary points :

S1. The coordinates for the adsorption of 1-butene on HZSM-23

O-O_2	-1	3.29007	3.95874	-4.95187	L			
O-O_2	-1	-3.33808	3.90375	-4.95837	L			
Si-Si3	-1	-0.01685	3.17755	-5.98797	L			
Si-Si3	-1	-2.92423	2.59327	-5.7257	L			
O-O_2	-1	-3.5467	1.28608	-5.11008	L			
O-O_2	-1	-1.32507	2.3509	-5.60314	L			
Si-Si3	-1	2.89888	2.64158	-5.71999	L			
O-O_2	-1	3.54174	1.3449	-5.10313	L			
O-O_2	-1	1.30437	2.37271	-5.60057	L			
O-O_2	-1	-0.02908	4.56604	-5.25836	L			
O-O_2	-1	-3.34916	4.97235	-2.70052	L			
O-O_2	-1	3.26782	6.10194	-0.42344	L	H-H_	28	0. 0.
O-O_2	-1	3.279	5.02741	-2.69401	L	H-H_	28	0. 0.
O-O_2	-1	-3.3603	6.04696	-0.42999	L			
Si-Si3	-1	-0.03907	5.32077	-1.45959	L			
Si-Si3	-1	-0.0414	5.96545	-4.53614	L			
Si-Si3	-1	6.28701	1.40849	-2.34827	L	H-H_	169	0. 0.
Si-Si3	-1	7.07507	4.06664	-3.60254	L			
O-O_2	-1	7.149	2.62369	-2.91924	L			
O-O_2	-1	5.61821	4.60506	-3.86451	L			
Si-Si3	-1	-6.29731	1.30397	-2.36063	L			
Si-Si3	-1	-7.12763	3.9488	-3.61646	L			
O-O_2	-1	-7.1783	2.50482	-2.93329	L			
O-O_2	-1	-5.6794	4.51133	-3.87559	L			
Si-Si3	-1	-2.94645	4.73648	-1.19732	L			
O-O_2	-1	-3.56892	3.4293	-0.5817	L			
O-O_2	-1	-1.34729	4.49412	-1.07476	L			
Si-Si3	-1	2.87671	4.78476	-1.19183	H			
O-O_2	-1	3.51938	3.48793	-0.57413	H			
O-O_2	-1	1.28217	4.51581	-1.0723	L	H-H_	28	0. 0.
Si-Si3	-1	-4.16734	4.92105	-4.06209	L			
Si-Si3	-1	-2.79174	7.33912	-5.19977	L			
O-O_2	-1	-1.36471	6.73526	-4.90697	L			
O-O_2	-1	-3.99992	6.37839	-4.751	L			
Si-Si3	-1	4.10057	4.98965	-4.05398	L			
Si-Si3	-1	2.68728	7.38458	-5.1944	L			
O-O_2	-1	1.26925	6.75711	-4.90439	L			
O-O_2	-1	3.91035	6.44402	-4.74324	L			
O-O_2	-1	-0.04019	5.6368	-2.99598	L			

O-O_2	-1	-0.05131	6.70926	-0.72998	L				
O-O_2	-1	-3.37138	7.11557	1.82786	L				
O-O_2	-1	3.25676	7.17056	1.83436	L				
Si-Si3	-1	-0.06129	7.46399	3.0688	L				
Si-Si3	-1	-0.06362	8.10867	-0.00776	L				
Si-Si3	-1	6.26473	3.55174	2.18	L	H-H_	172	0.	0.
Si-Si3	-1	7.05285	6.20986	0.92585	L				
O-O_2	-1	7.12677	4.7669	1.60914	L				
O-O_2	-1	5.59599	6.74828	0.66387	L				
Si-Si3	-1	-6.31954	3.44719	2.16775	L				
Si-Si3	-1	-7.14986	6.09202	0.91192	L				
O-O_2	-1	-7.20053	4.64803	1.59509	L				
O-O_2	-1	-5.70162	6.65454	0.65279	L				
Si-Si3	-1	-2.96867	6.8797	3.33106	L				
O-O_2	-1	-3.59114	5.57252	3.94668	L				
O-O_2	-1	-1.36951	6.63733	3.45362	L				
Si-Si3	-1	2.85443	6.92801	3.33677	L				
O-O_2	-1	3.4973	5.63133	3.95363	L				
O-O_2	-1	1.25992	6.65915	3.4562	L				
Si-Si3	-1	-4.18956	7.06427	0.46629	L				
Si-Si3	-1	-2.81396	9.48234	-0.67139	L				
O-O_2	-1	-1.38693	8.87848	-0.37859	L				
O-O_2	-1	-4.02214	8.5216	-0.22262	L				
Si-Si3	-1	4.07835	7.13287	0.4744	L				
Si-Si3	-1	2.66505	9.52779	-0.66602	L				
O-O_2	-1	1.24702	8.90033	-0.37601	L				
O-O_2	-1	3.88812	8.58723	-0.21486	L				
O-O_2	-1	-0.06241	7.78001	1.5324	L				
O-O_2	-1	8.03693	-7.18579	-2.42934	L				
O-O_2	-1	-7.91543	-6.24601	-0.17987	L				
O-O_2	-1	-7.42009	-2.47329	-1.968	L				
O-O_2	-1	-2.75283	-3.45437	-4.24831	L				
O-O_2	-1	-3.24814	-7.23051	-2.46743	L				
O-O_2	0	2.81459	-2.33589	-1.97845	H				
O-O_2	-1	3.36893	-6.10098	-0.19039	L				
O-O_2	-1	2.82496	-3.40809	-4.24284	L				
O-O_2	-1	3.38	-7.17552	-2.46093	L				
O-O_2	-1	-2.76395	-2.38333	-1.98509	H				
O-O_2	-1	-3.25929	-6.15591	-0.1969	L				
O-O_2	-1	-7.90431	-7.31805	-2.44497	L				
O-O_2	-1	8.02581	-6.11375	-0.16424	L				
O-O_2	-1	7.47145	-2.34974	-1.9534	L				
Si-Si3	-1	0.06183	-6.88213	-1.22644	L	H-H_	117	0.	0.
Si-Si3	-1	0.05961	-6.23742	-4.30305	L				

Si-Si3	-1	7.17609	-8.13623	-3.36944	L				
O-O_2	-1	5.71923	-7.59811	-3.63127	L				
Si-Si3	-1	-7.02662	-8.25406	-3.38337	L				
O-O_2	-1	-5.57838	-7.69184	-3.64235	L				
Si-Si3	-1	-4.46085	0.12678	-4.56589	L				
Si-Si3	-1	-3.63061	-2.51824	-3.30987	L	H-H_	77	0.	0.
Si-Si3	-1	-2.84543	-7.46669	-0.96408	L				
O-O_2	-1	-3.57986	-1.07436	-3.99308	L				
O-O_2	-1	-5.07877	-3.08057	-3.05093	L				
O-O_2	-1	-1.24628	-7.70875	-0.84167	L				
Si-Si3	-1	4.47394	0.20091	-4.55713	L				
Si-Si3	-1	3.6853	-2.45842	-3.303	L	H-H_	73	0.	0.
Si-Si3	-1	2.97767	-7.41838	-0.95837	L				
O-O_2	-1	3.61187	-1.0147	-3.98603	L				
O-O_2	-1	5.14266	-2.99577	-3.0409	L				
O-O_2	-1	1.38316	-7.68694	-0.83909	L				
Si-Si3	-1	6.66094	-3.38066	-2.85129	L				
Si-Si3	-1	8.07424	-5.77528	-1.71101	L				
O-O_2	-1	6.85052	-4.83472	-2.16217	L				
Si-Si3	-1	-6.59083	-3.4906	-2.86429	L				
Si-Si3	-1	-7.96643	-5.90836	-1.72675	L				
O-O_2	-1	-6.75825	-4.94763	-2.17552	L				
Si-Si3	-1	-4.06632	-7.28181	-3.829	L				
Si-Si3	-1	-2.69072	-4.86405	-4.96654	L				
O-O_2	-1	-1.26369	-5.46791	-4.67374	L				
O-O_2	-1	-3.8989	-5.82478	-4.51777	L				
Si-Si3	-1	4.20159	-7.21321	-3.82089	L				
Si-Si3	-1	2.7883	-4.81859	-4.96116	L				
O-O_2	-1	1.37026	-5.44605	-4.67115	L				
O-O_2	-1	4.01136	-5.75915	-4.51001	L				
O-O_2	-1	-5.37908	0.71528	-3.46321	L				
O-O_2	-1	5.38076	0.80455	-3.45266	L				
O-O_2	-1	0.06083	-6.56595	-2.76184	L				
O-O_2	-1	0.0499	-5.49376	-0.49673	H				
O-O_2	-1	8.01471	-5.043	2.09814	L				
O-O_2	-1	7.46032	-1.27516	0.31714	L				
O-O_2	-1	-7.93765	-4.1028	4.34851	L				
O-O_2	-1	-7.44231	-0.33007	2.56038	L				
O-O_2	-1	-2.7752	-1.31074	0.28083	H				
O-O_2	-1	-3.27036	-5.0873	2.06095	L				
O-O_2	0	2.60369	-0.19841	2.58583	H				
O-O_2	-1	3.34664	-3.9577	4.33798	L				
O-O_3	0	2.56865	-1.27566	0.2572	H				
O-O_2	-1	3.35781	-5.03242	2.06747	L				

O-O_2	-1	-2.78598	-0.23993	2.5433	H				
O-O_2	-1	-3.28151	-4.01269	4.33148	L				
O-O_2	-1	-7.92653	-5.17526	2.08251	L				
O-O_2	-1	-7.43123	-1.39868	0.30253	L				
O-O_2	-1	8.00359	-3.97053	4.36414	L				
O-O_2	-1	7.44923	-0.20655	2.575	L				
Si-Si3	-1	0.0397	-4.73893	3.30188	L	H-H_	173	0.	0.
Si-Si3	-1	0.03819	-4.13602	0.24131	H				
Si-Si3	-1	7.15386	-5.99301	1.15894	L				
Si-Si3	-1	7.86199	-1.03229	-1.18542	L				
O-O_2	-1	7.21913	0.2641	-1.80214	L				
O-O_2	-1	5.69701	-5.45492	0.89705	L				
Si-Si3	-1	-7.04884	-6.11085	1.14501	L				
Si-Si3	-1	-7.83394	-1.16251	-1.20082	L				
O-O_2	-1	-7.21147	0.14437	-1.81629	L				
O-O_2	-1	-5.6006	-5.54863	0.88603	L				
Si-Si3	-1	-4.48308	2.27	-0.03751	L				
Si-Si3	-1	-3.65278	-0.37518	1.21837	H				
Si-Si3	-1	-2.86766	-5.32347	3.5643	L				
O-O_2	-1	-3.60206	1.06885	0.53529	L	H-H_	145	0.	0.
O-O_2	-1	-5.10098	-0.9373	1.4776	L	H-H_	145	0.	0.
O-O_2	-1	-1.2685	-5.56554	3.68671	L				
Si-Si3	0	4.43804	2.32388	-0.02118	H				
Si-Si3	-1	2.95545	-5.27516	3.57001	L				
O-O_2	0	3.36782	1.23844	0.38819	H				
O-O_2	0	5.11098	-0.87524	1.42283	H				
O-O_2	-1	1.36094	-5.54372	3.68929	L				
Si-Si3	-1	6.63866	-1.23735	1.67701	L	H-H_	153	0.	0.
Si-Si3	-1	8.05201	-3.63206	2.81737	L				
O-O_2	-1	6.8283	-2.69151	2.36621	L				
Si-Si3	-1	-6.61305	-1.34739	1.66409	L				
Si-Si3	-1	-7.98865	-3.76515	2.80164	L				
O-O_2	-1	-6.78048	-2.80441	2.35286	L				
Si-Si3	-1	-4.08854	-5.1386	0.69939	L				
Si-Si3	-1	-2.71273	-2.72106	-0.43807	H				
O-O_2	-1	-1.25742	-3.30884	-0.14187	H				
O-O_2	-1	-3.92115	-3.68151	0.01065	L	H-H_	162	0.	0.
Si-Si3	-1	4.1791	-5.06956	0.70737	L	H-H_	168	0.	0.
Si-Si3	0	2.81309	-2.74551	-0.46212	H				
O-O_2	0	1.43555	-3.4608	-0.14664	H				
O-O_2	0	4.12449	-3.54639	0.01927	H				
O-O_2	-1	5.36934	1.87611	-1.1884	H				
O-O_2	-1	-5.4013	2.85849	1.06517	L				
O-O_2	-1	-5.39019	1.78689	-1.19902	L				

O-O_2	-1	5.35853	2.94728	1.07564	H				
O-O_2	-1	0.03855	-4.42299	1.76522	H				
O-O_2	-1	0.02749	-3.35069	4.03164	L				
O-O_2	-1	7.43809	0.86809	4.84551	L				
O-O_2	-1	-2.79729	0.8325	4.80936	L				
O-O_2	-1	2.78082	0.87902	4.81414	H				
O-O_2	-1	-7.45345	0.74453	4.83091	L				
Si-Si3	-1	0.01509	-1.95048	4.7545	L	H-H_	204	0.	0.
Si-Si3	-1	7.13164	-3.84979	5.68732	L				
Si-Si3	-1	7.83977	1.11093	3.34296	L				
O-O_2	-1	7.19691	2.40731	2.72624	L				
O-O_2	-1	5.67478	-3.31168	5.42549	L				
Si-Si3	-1	-7.07106	-3.96763	5.67339	L				
Si-Si3	-1	-7.85616	0.98071	3.32756	L				
O-O_2	-1	-7.23369	2.28759	2.71209	L				
O-O_2	-1	-5.62282	-3.40541	5.41441	L				
Si-Si3	-1	-4.5053	4.41322	4.49087	L				
Si-Si3	-1	-3.67497	1.76808	5.74685	L				
O-O_2	-1	-3.62431	3.21207	5.06368	L				
O-O_2	-1	-5.12321	1.20586	6.00583	L				
Si-Si3	-1	4.42949	4.48735	4.49963	L				
Si-Si3	-1	3.64114	1.8286	5.75441	L	H-H_	177	0.	0.
O-O_2	-1	3.56743	3.27174	5.07073	L				
O-O_2	-1	5.09821	1.29067	6.01586	L				
Si-Si3	-1	6.6165	0.90578	6.20547	L				
Si-Si3	-1	-6.63527	0.79583	6.19247	L				
Si-Si3	-1	-4.11077	-2.99538	5.22776	L				
Si-Si3	-1	-2.73516	-0.5776	4.09023	L	H-H_	128	0.	0.
O-O_2	-1	-1.30814	-1.18147	4.38302	L				
O-O_2	-1	-3.94334	-1.53835	4.539	L				
Si-Si3	-1	4.15713	-2.92685	5.23574	L	H-H_	205	0.	0.
Si-Si3	0	2.73348	-0.54653	4.11672	H				
O-O_2	-1	1.32586	-1.16056	4.38434	H				
O-O_2	-1	3.96698	-1.47232	4.54715	H				
O-O_2	-1	5.34742	4.01937	3.33991	L				
O-O_2	-1	-5.41242	3.9301	3.32936	L				
H-H_	-1	-7.07322	-9.58218	-2.75502	L				
H-H_	-1	-7.09545	-7.43897	1.77336	L				
H-H_	-1	-7.11767	-5.29575	6.30174	L				
H-H_	-1	-3.42716	-8.68802	-0.3889	L				
H-H_	-1	-3.44938	-6.54481	4.13948	L				
H-H_	-1	3.57846	-8.6299	-0.38203	L				
H-H_	-1	3.55623	-6.48668	4.14635	L				
H-H_	-1	7.22186	-7.32016	1.78739	L				

H-H_	-1	7.19963	-5.17694	6.31577	L
H-H_	-1	7.9279	-2.97106	6.55605	L
H-H_	-1	-9.28323	-0.94313	-1.31176	L
H-H_	-1	-7.34758	-3.53805	-4.12364	L
H-H_	-1	-9.29667	-5.34546	-1.99969	L
H-H_	-1	-7.82837	-8.37912	-4.60912	L
H-H_	-1	-7.92938	3.82375	-4.84222	L
H-H_	-1	-7.93965	4.81439	-2.74911	L
H-H_	-1	-5.32064	-0.33112	-5.6668	L
H-H_	-1	-9.30546	1.20009	3.21662	L
H-H_	-1	-9.31889	-3.20225	2.52869	L
H-H_	-1	-7.96188	6.9576	1.77927	L
H-H_	-1	-7.9516	5.96697	-0.31383	L
H-H_	-1	-2.87161	10.79076	-0.00385	L
H-H_	-1	7.24408	-9.46338	-2.74099	L
H-H_	-1	9.39549	-5.19038	-1.98136	L
H-H_	-1	9.37327	-3.04716	2.54702	L
H-H_	-1	9.30764	-0.7888	-1.29357	L
H-H_	-1	9.28542	1.35442	3.23481	L
H-H_	-1	7.84911	7.08859	1.79458	L
H-H_	-1	7.85938	6.09818	-0.29806	L
H-H_	-1	7.87133	4.94538	-2.7338	L
H-H_	-1	7.8816	3.95496	-4.82644	L
H-H_	-1	-2.86129	9.79542	-2.10689	L
H-H_	-1	-2.84939	8.64754	-4.53223	L
H-H_	-1	-2.83907	7.6522	-6.63527	L
H-H_	-1	2.73162	7.69843	-6.62982	L
H-H_	-1	2.7213	8.69378	-4.52676	L
H-H_	-1	2.7094	9.84164	-2.10144	L
H-H_	-1	2.69908	10.83699	0.00162	L
H-H_	-1	-7.40228	1.73677	7.02147	L
H-H_	-1	-5.37562	4.97101	5.53601	L
H-H_	-1	-3.35518	8.1036	4.0477	L
H-H_	-1	-2.87363	1.89347	6.97283	L
H-H_	-1	-0.07276	8.76549	3.75205	L
H-H_	-1	2.83522	1.94081	6.97816	L
H-H_	-1	3.21974	8.15803	4.05407	L
H-H_	-1	5.28878	5.05935	5.54622	L
H-H_	-1	7.36616	1.8593	7.03595	L
H-H_	-1	3.27459	2.86808	-7.123	L
H-H_	-1	5.34376	-0.24253	-5.65607	L
H-H_	-1	7.42085	-3.41552	-4.10916	L
H-H_	-1	7.98262	-8.24791	-4.59334	L
H-H_	-1	2.83263	-4.5045	-6.39653	L

H-H_	-1	3.45193	-8.16674	-4.65137	L
H-H_	-1	0.07111	-7.54378	-4.97697	L
H-H_	-1	-2.73804	-4.55073	-6.40198	L
H-H_	-1	-3.29932	-8.22275	-4.65799	L
H-H_	-1	-7.88308	-3.10205	6.54074	L
H-H_	-1	-6.78717	-0.52604	6.81735	L
H-H_	-1	-3.30033	2.81355	-7.1296	L
H-H_	-1	-0.0179	3.47427	-7.42771	L
H-H_	-1	0.01631	-2.258	6.1913	L
H-H_	-1	3.39724	-2.89192	6.49374	L
H-H_	-1	6.7885	-0.41347	6.83069	L
H-H_	-1	-3.35401	-2.94793	6.48712	L
Al-Al3	0	3.60354	-0.17269	1.26305	H
H-H_	0	0.73578	1.24069	-1.11172	H
C-C_2	0	0.14326	0.58413	-0.47957	H
C-C_2	0	-0.07389	0.86969	0.81401	H
H-H_	0	-0.32767	-0.27512	-0.95194	H
H-H_	0	1.70714	-0.81735	0.09098	H
H-H_	0	-0.68308	0.18571	1.4021	H
C-C_3	0	0.41492	2.0854	1.54979	H
C-C_3	0	-0.74466	2.91446	2.13341	H
H-H_	0	1.03441	2.69691	0.88908	H
H-H_	0	1.06534	1.75142	2.36594	H
H-H_	0	-0.36061	3.77137	2.69702	H
H-H_	0	-1.40248	3.29818	1.34799	H
H-H_	0	-1.3607	2.3134	2.81013	H

S2. The coordinates for INT1 on HZSM-23

O-O_2	-1	3.38279	3.84429	-4.98754	L			
O-O_2	-1	-3.24397	3.99045	-4.97667	L			
Si-Si3	-1	0.05094	3.16137	-6.01312	L			
Si-Si3	-1	-2.87212	2.6662	-5.74186	L			
O-O_2	-1	-3.53232	1.37998	-5.12143	L			
O-O_2	-1	-1.28073	2.37571	-5.62287	L			
Si-Si3	-1	2.94977	2.53779	-5.75141	L			
O-O_2	-1	3.55464	1.22367	-5.13305	L			
O-O_2	-1	1.34816	2.31773	-5.62718	L			
O-O_2	-1	0.08279	4.55132	-5.28689	L			
O-O_2	-1	-3.21658	5.06426	-2.72143	L			
O-O_2	-1	3.43768	5.99791	-0.46434	L	H-H_	28	0. 0.
O-O_2	-1	3.41019	4.91816	-2.73228	L	H-H_	28	0. 0.
O-O_2	-1	-3.18905	6.14409	-0.45352	L			
Si-Si3	-1	0.10586	5.315	-1.48996	L			
Si-Si3	-1	0.11486	5.95216	-4.56807	L			

Si-Si3	-1	6.30793	1.21045	-2.3855	L	H-H_	169	0.	0.
Si-Si3	-1	7.17292	3.84049	-3.64832	L				
O-O_2	-1	7.20486	2.39758	-2.96169	L				
O-O_2	-1	5.73237	4.42224	-3.90783	L				
Si-Si3	-1	-6.27376	1.48785	-2.36488	L				
Si-Si3	-1	-7.02681	4.15367	-3.62503	L				
O-O_2	-1	-7.11944	2.71351	-2.93819	L				
O-O_2	-1	-5.56287	4.67137	-3.8893	L				
Si-Si3	-1	-2.8172	4.81984	-1.21871	L				
O-O_2	-1	-3.4774	3.53361	-0.59827	L				
O-O_2	-1	-1.22581	4.52935	-1.09971	L				
Si-Si3	-1	3.00474	4.6914	-1.22846	H				
O-O_2	-1	3.60942	3.37712	-0.60929	H				
O-O_2	-1	1.4031	4.47124	-1.10414	L	H-H_	28	0.	0.
Si-Si3	-1	-4.03958	5.03458	-4.08073	L				
Si-Si3	-1	-2.5943	7.40708	-5.22791	L				
O-O_2	-1	-1.18547	6.7609	-4.93735	L				
O-O_2	-1	-3.82986	6.48453	-4.77365	L				
Si-Si3	-1	4.2266	4.85227	-4.09429	L				
Si-Si3	-1	2.88357	7.28626	-5.2369	L				
O-O_2	-1	1.44794	6.70281	-4.94167	L				
O-O_2	-1	4.07874	6.31009	-4.78662	L				
O-O_2	-1	0.11022	5.62728	-3.02712	L				
O-O_2	-1	0.13771	6.70495	-0.76373	L				
O-O_2	-1	-3.16166	7.21789	1.80173	L				
O-O_2	-1	3.46509	7.07173	1.79086	L				
Si-Si3	-1	0.16078	7.46864	3.03319	L				
Si-Si3	-1	0.16978	8.1058	-0.04491	L				
Si-Si3	-1	6.36279	3.36413	2.13754	L	H-H_	172	0.	0.
Si-Si3	-1	7.22784	5.99412	0.87483	L				
O-O_2	-1	7.25978	4.55121	1.56147	L				
O-O_2	-1	5.78729	6.57588	0.61533	L				
Si-Si3	-1	-6.21884	3.64148	2.15828	L				
Si-Si3	-1	-6.97189	6.30731	0.89812	L				
O-O_2	-1	-7.06452	4.86715	1.58496	L				
O-O_2	-1	-5.50795	6.82501	0.63386	L				
Si-Si3	-1	-2.76228	6.97348	3.30445	L				
O-O_2	-1	-3.42248	5.68725	3.92489	L				
O-O_2	-1	-1.17089	6.68298	3.42344	L				
Si-Si3	-1	3.0596	6.84507	3.2949	L				
O-O_2	-1	3.66448	5.53094	3.91326	L				
O-O_2	-1	1.458	6.625	3.41913	L				
Si-Si3	-1	-3.98466	7.18822	0.44242	L				
Si-Si3	-1	-2.53937	9.56072	-0.70476	L				

O-O_2	-1	-1.13055	8.91453	-0.41419	L			
O-O_2	-1	-3.77494	8.63816	-0.25049	L			
Si-Si3	-1	4.28152	7.0059	0.42886	L			
Si-Si3	-1	2.93849	9.4399	-0.71374	L			
O-O_2	-1	1.50286	8.85645	-0.41851	L			
O-O_2	-1	4.13366	8.46373	-0.26347	L			
O-O_2	-1	0.16515	7.78091	1.49604	L			
O-O_2	-1	7.79607	-7.43314	-2.45005	L			
O-O_2	-1	-8.11436	-6.00436	-0.16142	L			
O-O_2	-1	-7.50957	-2.25266	-1.96008	L			
O-O_2	-1	-2.88034	-3.38033	-4.25011	L			
O-O_2	-1	-3.48523	-7.13547	-2.45869	L			
O-O_2	0	2.73724	-2.35271	-1.99052	H			
O-O_2	-1	3.16913	-6.20186	-0.20164	L			
O-O_2	-1	2.69628	-3.50332	-4.25925	L			
O-O_2	-1	3.14153	-7.28163	-2.46955	L			
O-O_2	-1	-2.8529	-2.30408	-1.98949	H			
O-O_2	-1	-3.45769	-6.05564	-0.19078	L			
O-O_2	-1	-8.14184	-7.08161	-2.42391	L			
O-O_2	-1	7.82354	-6.35589	-0.18757	L			
O-O_2	-1	7.37885	-2.58104	-1.9845	L			
Si-Si3	-1	-0.1629	-6.88475	-1.22716	L	H-H_	117	0. 0.
Si-Si3	-1	-0.15378	-6.24756	-4.30533	L			
Si-Si3	-1	6.90427	-8.35924	-3.38558	L			
O-O_2	-1	5.46372	-7.77778	-3.64494	L			
Si-Si3	-1	-7.29546	-8.04605	-3.36229	L			
O-O_2	-1	-5.83152	-7.52866	-3.62642	L			
Si-Si3	-1	-4.47977	0.25025	-4.57202	L			
Si-Si3	-1	-3.7268	-2.41577	-3.31168	L	H-H_	77	0. 0.
Si-Si3	-1	-3.08585	-7.38019	-0.95582	L			
O-O_2	-1	-3.63409	-0.97572	-3.99856	L			
O-O_2	-1	-5.19066	-2.93328	-3.0476	L			
O-O_2	-1	-1.49446	-7.67038	-0.83697	L			
Si-Si3	-1	4.45315	0.05322	-4.58667	L			
Si-Si3	-1	3.58755	-2.57797	-3.32397	L	H-H_	73	0. 0.
Si-Si3	-1	2.73603	-7.5086	-0.96537	L			
O-O_2	-1	3.55613	-1.13431	-4.01035	L			
O-O_2	-1	5.02863	-3.15868	-3.06436	L			
O-O_2	-1	1.13443	-7.72837	-0.84128	L			
Si-Si3	-1	6.53504	-3.58901	-2.87775	L			
Si-Si3	-1	7.87807	-6.02271	-1.73528	L			
O-O_2	-1	6.68226	-5.04652	-2.18556	L			
Si-Si3	-1	-6.71395	-3.29679	-2.85602	L			
Si-Si3	-1	-8.15923	-5.66899	-1.70898	L			

O-O_2	-1	-6.92367	-4.74643	-2.16325	L			
Si-Si3	-1	-4.30823	-7.16514	-3.81799	L			
Si-Si3	-1	-2.86295	-4.79294	-4.96503	L			
O-O_2	-1	-1.45412	-5.43913	-4.67446	L			
O-O_2	-1	-4.09851	-5.7155	-4.51076	L			
Si-Si3	-1	3.95795	-7.34746	-3.83155	L			
Si-Si3	-1	2.61492	-4.91377	-4.97401	L			
O-O_2	-1	1.17928	-5.49721	-4.67878	L			
O-O_2	-1	3.81009	-5.88994	-4.52374	L			
O-O_2	-1	-5.37677	0.86895	-3.4684	L			
O-O_2	-1	5.38082	0.63168	-3.48604	L			
O-O_2	-1	-0.15842	-6.57232	-2.76333	L			
O-O_2	-1	-0.13075	-5.49493	-0.50083	H			
O-O_2	-1	7.85098	-5.27993	2.0722	L			
O-O_2	-1	7.40639	-1.50124	0.28342	L			
O-O_2	-1	-8.05945	-3.85073	4.36173	L			
O-O_2	-1	-7.45465	-0.09902	2.56308	L			
O-O_2	-1	-2.82555	-1.22628	0.27381	H			
O-O_2	-1	-3.43031	-4.98183	2.06447	L			
O-O_2	0	2.5063	-0.00634	2.57132	H			
O-O_2	-1	3.22398	-4.04816	4.32151	L			
O-O_3	0	2.52798	-1.53494	0.41704	H			
O-O_2	-1	3.19647	-5.12811	2.05362	L			
O-O_2	-1	-2.79779	-0.15027	2.53367	H			
O-O_2	-1	-3.40277	-3.902	4.33238	L			
O-O_2	-1	-8.08693	-4.92841	2.09835	L			
O-O_2	-1	-7.48203	-1.17283	0.30783	L			
O-O_2	-1	7.87846	-4.20225	4.33559	L			
O-O_2	-1	7.43377	-0.42743	2.53868	L			
Si-Si3	-1	-0.10789	-4.73114	3.29592	L	H-H_	173	0. 0.
Si-Si3	-1	-0.09929	-4.13572	0.23388	H			
Si-Si3	-1	6.95919	-6.2056	1.13758	L			
Si-Si3	-1	7.81123	-1.27423	-1.22077	L			
O-O_2	-1	7.20635	0.0396	-1.83899	L			
O-O_2	-1	5.51864	-5.62417	0.87816	L			
Si-Si3	-1	-7.24054	-5.89242	1.16087	L			
Si-Si3	-1	-7.88141	-0.92811	-1.19504	L			
O-O_2	-1	-7.22122	0.35782	-1.81533	L			
O-O_2	-1	-5.7766	-5.37502	0.89674	L			
Si-Si3	-1	-4.42484	2.40388	-0.04886	L			
Si-Si3	-1	-3.67184	-0.26229	1.21134	H			
Si-Si3	-1	-3.03093	-5.22656	3.56734	L			
O-O_2	-1	-3.57915	1.17791	0.52459	L	H-H_	145	0. 0.
O-O_2	-1	-5.13573	-0.77959	1.47571	L	H-H_	145	0. 0.

O-O_2	-1	-1.43954	-5.51674	3.68618	L				
Si-Si3	0	4.48512	2.17946	-0.05103	H				
Si-Si3	-1	2.79095	-5.35496	3.55779	L				
O-O_2	0	3.42649	1.10798	0.42671	H				
O-O_2	0	5.07028	-1.03745	1.43108	H				
O-O_2	-1	1.18935	-5.57473	3.68187	L				
Si-Si3	-1	6.5899	-1.43529	1.64533	L	H-H_	153	0.	0.
Si-Si3	-1	7.93299	-3.86908	2.78787	L				
O-O_2	-1	6.73717	-2.89289	2.33759	L				
Si-Si3	-1	-6.65903	-1.14316	1.66714	L				
Si-Si3	-1	-8.10431	-3.51535	2.81418	L				
O-O_2	-1	-6.86875	-2.5928	2.35991	L				
Si-Si3	-1	-4.25331	-5.01151	0.70516	L				
Si-Si3	-1	-2.80783	-2.63955	-0.44181	H				
O-O_2	-1	-1.37023	-3.27049	-0.14788	H				
O-O_2	-1	-4.04362	-3.56181	0.01242	L	H-H_	162	0.	0.
Si-Si3	-1	4.01262	-5.19338	0.69149	L	H-H_	168	0.	0.
Si-Si3	0	2.7209	-2.83617	-0.46308	H				
O-O_2	0	1.32326	-3.59607	-0.23444	H				
O-O_2	0	4.03779	-3.72452	-0.05473	H				
O-O_2	-1	5.40796	1.70846	-1.22439	H				
O-O_2	-1	-5.32184	3.02258	1.05476	L				
O-O_2	-1	-5.3493	1.94576	-1.20682	L				
O-O_2	-1	5.43572	2.78483	1.03704	H				
O-O_2	-1	-0.10356	-4.41895	1.75851	H				
O-O_2	-1	-0.07603	-3.34144	4.02231	L				
O-O_2	-1	7.4613	0.65243	4.80657	L				
O-O_2	-1	-2.77049	0.92738	4.79711	L				
O-O_2	-1	2.80646	0.80463	4.78728	H				
O-O_2	-1	-7.42711	0.98081	4.83099	L				
Si-Si3	-1	-0.04401	-1.93975	4.74181	L	H-H_	204	0.	0.
Si-Si3	-1	7.01411	-4.05197	5.66073	L				
Si-Si3	-1	7.86615	0.87941	3.30238	L				
O-O_2	-1	7.26127	2.19324	2.68417	L				
O-O_2	-1	5.57355	-3.47051	5.40137	L				
Si-Si3	-1	-7.18562	-3.73878	5.68402	L				
Si-Si3	-1	-7.82649	1.22553	3.32812	L				
O-O_2	-1	-7.1663	2.51145	2.70783	L				
O-O_2	-1	-5.72168	-3.22139	5.4199	L				
Si-Si3	-1	-4.36993	4.55752	4.47429	L				
Si-Si3	-1	-3.61688	1.89139	5.73459	L				
O-O_2	-1	-3.52426	3.33155	5.04775	L				
O-O_2	-1	-5.08082	1.374	5.99872	L				
Si-Si3	-1	4.56299	4.36049	4.45964	L				

Si-Si3	-1	3.69769	1.72987	5.72299	L	H-H_	177	0.	0.
O-O_2	-1	3.66597	3.17296	5.03596	L				
O-O_2	-1	5.13847	1.1486	5.98196	L				
Si-Si3	-1	6.64488	0.71826	6.16856	L				
Si-Si3	-1	-6.60412	1.01048	6.19029	L				
Si-Si3	-1	-4.19839	-2.85787	5.22832	L				
Si-Si3	-1	-2.7531	-0.48566	4.08129	L	H-H_	128	0.	0.
O-O_2	-1	-1.34428	-1.13186	4.37185	L				
O-O_2	-1	-3.98868	-1.40823	4.53555	L				
Si-Si3	-1	4.06777	-3.04026	5.21461	L	H-H_	205	0.	0.
Si-Si3	0	2.71569	-0.62527	4.12593	H				
O-O_2	-1	1.28914	-1.19094	4.3662	H				
O-O_2	-1	3.92	-1.58224	4.523	H				
O-O_2	-1	5.4632	3.86213	3.29869	L				
O-O_2	-1	-5.29438	4.0994	3.31633	L				
H-H_	-1	-7.38065	-9.37065	-2.73057	L				
H-H_	-1	-7.32574	-7.21702	1.79259	L				
H-H_	-1	-7.27081	-5.06338	6.31575	L				
H-H_	-1	-3.70283	-8.58194	-0.37613	L				
H-H_	-1	-3.64791	-6.4283	4.14703	L				
H-H_	-1	3.30132	-8.73643	-0.38762	L				
H-H_	-1	3.35624	-6.58279	4.13554	L				
H-H_	-1	6.98857	-7.53271	1.7691	L				
H-H_	-1	7.04349	-5.37908	6.29226	L				
H-H_	-1	7.83899	-3.19575	6.52524	L				
H-H_	-1	-9.32367	-0.66511	-1.30275	L				
H-H_	-1	-7.47517	-3.32424	-4.11328	L				
H-H_	-1	-9.47251	-5.06663	-1.97984	L				
H-H_	-1	-8.1039	-8.14962	-4.58564	L				
H-H_	-1	-7.83526	4.05011	-4.84838	L				
H-H_	-1	-7.80987	5.04555	-2.7577	L				
H-H_	-1	-5.35599	-0.18397	-5.66956	L				
H-H_	-1	-9.26875	1.48852	3.22041	L				
H-H_	-1	-9.41759	-2.91299	2.54331	L				
H-H_	-1	-7.75495	7.19919	1.76546	L				
H-H_	-1	-7.78034	6.20374	-0.32523	L				
H-H_	-1	-2.55552	10.87187	-0.04028	L				
H-H_	-1	6.93365	-9.68635	-2.75405	L				
H-H_	-1	9.21573	-5.47882	-2.0105	L				
H-H_	-1	9.27065	-3.32518	2.51266	L				
H-H_	-1	9.26331	-1.07498	-1.33328	L				
H-H_	-1	9.31823	1.07866	3.18988	L				
H-H_	-1	8.05271	6.85034	1.73934	L				
H-H_	-1	8.02733	5.85511	-0.35088	L				

H-H_	-1	7.99779	4.69671	-2.78382	L
H-H_	-1	7.97242	3.70148	-4.87404	L
H-H_	-1	-2.58102	9.87169	-2.14089	L
H-H_	-1	-2.61044	8.71823	-4.56343	L
H-H_	-1	-2.63594	7.71805	-6.66404	L
H-H_	-1	2.93358	7.59522	-6.67319	L
H-H_	-1	2.95909	8.5954	-4.57256	L
H-H_	-1	2.9885	9.74885	-2.15004	L
H-H_	-1	3.01401	10.74904	-0.04941	L
H-H_	-1	-7.34	1.97623	7.01897	L
H-H_	-1	-5.22012	5.14394	5.52033	L
H-H_	-1	-3.10956	8.21024	4.01909	L
H-H_	-1	-2.80883	1.9953	6.95817	L
H-H_	-1	0.19063	8.77151	3.71329	L
H-H_	-1	2.89882	1.86939	6.94854	L
H-H_	-1	3.46398	8.06513	4.00823	L
H-H_	-1	5.44204	4.90863	5.50258	L
H-H_	-1	7.42534	1.65056	6.99475	L
H-H_	-1	3.32842	2.74946	-7.15594	L
H-H_	-1	5.30618	-0.41902	-5.68678	L
H-H_	-1	7.29018	-3.6499	-4.1375	L
H-H_	-1	7.70377	-8.49825	-4.6113	L
H-H_	-1	2.66493	-4.60457	-6.41026	L
H-H_	-1	3.17749	-8.27976	-4.65774	L
H-H_	-1	-0.18373	-7.55527	-4.97608	L
H-H_	-1	-2.90458	-4.48173	-6.4011	L
H-H_	-1	-3.57234	-8.13089	-4.64667	L
H-H_	-1	-7.96868	-2.8469	6.55136	L
H-H_	-1	-6.79437	-0.30469	6.8188	L
H-H_	-1	-3.24512	2.89447	-7.14531	L
H-H_	-1	0.05504	3.45457	-7.45357	L
H-H_	-1	-0.04828	-2.24379	6.17931	L
H-H_	-1	3.31266	-2.9793	6.47451	L
H-H_	-1	6.77845	-0.60411	6.79657	L
H-H_	-1	-3.43717	-2.83043	6.48558	L
Al-Al3	0	3.56302	-0.42576	1.13536	H
H-H_	0	0.91622	0.42807	0.31433	H
C-C_3	0	0.417	0.32422	1.27751	H
C-C_3	0	1.27652	0.87064	2.40547	H
H-H_	0	-0.52025	0.88544	1.26388	H
H-H_	0	0.17464	-0.72786	1.4287	H
H-H_	0	0.73366	0.76381	3.34275	H
C-C_3	0	1.60428	2.3595	2.24049	H
C-C_3	0	0.45523	3.22613	2.77108	H

H-H_	0	1.79909	2.57465	1.19177	H
H-H_	0	2.52428	2.59153	2.77912	H
H-H_	0	0.64868	4.27911	2.55242	H
H-H_	0	-0.50104	2.97243	2.30149	H
H-H_	0	0.33038	3.12229	3.85562	H

S3. The coordinates for INT2 on HZSM-23

O-O_2	-1	3.29007	3.95874	-4.95187	L			
O-O_2	-1	-3.33808	3.90375	-4.95837	L			
Si-Si3	-1	-0.01685	3.17755	-5.98797	L			
Si-Si3	-1	-2.92423	2.59327	-5.7257	L			
O-O_2	-1	-3.5467	1.28608	-5.11008	L			
O-O_2	-1	-1.32507	2.3509	-5.60314	L			
Si-Si3	-1	2.89888	2.64158	-5.71999	L			
O-O_2	-1	3.54174	1.3449	-5.10313	L			
O-O_2	-1	1.30437	2.37271	-5.60057	L			
O-O_2	-1	-0.02908	4.56604	-5.25836	L			
O-O_2	-1	-3.34916	4.97235	-2.70052	L			
O-O_2	-1	3.26782	6.10194	-0.42344	L	H-H_	28	0. 0.
O-O_2	-1	3.279	5.02741	-2.69401	L	H-H_	28	0. 0.
O-O_2	-1	-3.3603	6.04696	-0.42999	L			
Si-Si3	-1	-0.03907	5.32077	-1.45959	L			
Si-Si3	-1	-0.0414	5.96545	-4.53614	L			
Si-Si3	-1	6.28701	1.40849	-2.34827	L	H-H_	169	0. 0.
Si-Si3	-1	7.07507	4.06664	-3.60254	L			
O-O_2	-1	7.149	2.62369	-2.91924	L			
O-O_2	-1	5.61821	4.60506	-3.86451	L			
Si-Si3	-1	-6.29731	1.30397	-2.36063	L			
Si-Si3	-1	-7.12763	3.9488	-3.61646	L			
O-O_2	-1	-7.1783	2.50482	-2.93329	L			
O-O_2	-1	-5.6794	4.51133	-3.87559	L			
Si-Si3	-1	-2.94645	4.73648	-1.19732	L			
O-O_2	-1	-3.56892	3.4293	-0.5817	L			
O-O_2	-1	-1.34729	4.49412	-1.07476	L			
Si-Si3	-1	2.87671	4.78476	-1.19183	H			
O-O_2	-1	3.51938	3.48793	-0.57413	H			
O-O_2	-1	1.28217	4.51581	-1.0723	L	H-H_	28	0. 0.
Si-Si3	-1	-4.16734	4.92105	-4.06209	L			
Si-Si3	-1	-2.79174	7.33912	-5.19977	L			
O-O_2	-1	-1.36471	6.73526	-4.90697	L			
O-O_2	-1	-3.99992	6.37839	-4.751	L			
Si-Si3	-1	4.10057	4.98965	-4.05398	L			
Si-Si3	-1	2.68728	7.38458	-5.1944	L			
O-O_2	-1	1.26925	6.75711	-4.90439	L			

O-O_2	-1	3.91035	6.44402	-4.74324	L				
O-O_2	-1	-0.04019	5.6368	-2.99598	L				
O-O_2	-1	-0.05131	6.70926	-0.72998	L				
O-O_2	-1	-3.37138	7.11557	1.82786	L				
O-O_2	-1	3.25676	7.17056	1.83436	L				
Si-Si3	-1	-0.06129	7.46399	3.0688	L				
Si-Si3	-1	-0.06362	8.10867	-0.00776	L				
Si-Si3	-1	6.26473	3.55174	2.18	L	H-H_	172	0.	0.
Si-Si3	-1	7.05285	6.20986	0.92585	L				
O-O_2	-1	7.12677	4.7669	1.60914	L				
O-O_2	-1	5.59599	6.74828	0.66387	L				
Si-Si3	-1	-6.31954	3.44719	2.16775	L				
Si-Si3	-1	-7.14986	6.09202	0.91192	L				
O-O_2	-1	-7.20053	4.64803	1.59509	L				
O-O_2	-1	-5.70162	6.65454	0.65279	L				
Si-Si3	-1	-2.96867	6.8797	3.33106	L				
O-O_2	-1	-3.59114	5.57252	3.94668	L				
O-O_2	-1	-1.36951	6.63733	3.45362	L				
Si-Si3	-1	2.85443	6.92801	3.33677	L				
O-O_2	-1	3.4973	5.63133	3.95363	L				
O-O_2	-1	1.25992	6.65915	3.4562	L				
Si-Si3	-1	-4.18956	7.06427	0.46629	L				
Si-Si3	-1	-2.81396	9.48234	-0.67139	L				
O-O_2	-1	-1.38693	8.87848	-0.37859	L				
O-O_2	-1	-4.02214	8.5216	-0.22262	L				
Si-Si3	-1	4.07835	7.13287	0.4744	L				
Si-Si3	-1	2.66505	9.52779	-0.66602	L				
O-O_2	-1	1.24702	8.90033	-0.37601	L				
O-O_2	-1	3.88812	8.58723	-0.21486	L				
O-O_2	-1	-0.06241	7.78001	1.5324	L				
O-O_2	-1	8.03693	-7.18579	-2.42934	L				
O-O_2	-1	-7.91543	-6.24601	-0.17987	L				
O-O_2	-1	-7.42009	-2.47329	-1.968	L				
O-O_2	-1	-2.75283	-3.45437	-4.24831	L				
O-O_2	-1	-3.24814	-7.23051	-2.46743	L				
O-O_2	0	2.81459	-2.33589	-1.97845	H				
O-O_2	-1	3.36893	-6.10098	-0.19039	L				
O-O_2	-1	2.82496	-3.40809	-4.24284	L				
O-O_2	-1	3.38	-7.17552	-2.46093	L				
O-O_2	-1	-2.76395	-2.38333	-1.98509	H				
O-O_2	-1	-3.25929	-6.15591	-0.1969	L				
O-O_2	-1	-7.90431	-7.31805	-2.44497	L				
O-O_2	-1	8.02581	-6.11375	-0.16424	L				
O-O_2	-1	7.47145	-2.34974	-1.9534	L				

Si-Si3	-1	0.06183	-6.88213	-1.22644	L	H-H_	117	0.	0.
Si-Si3	-1	0.05961	-6.23742	-4.30305	L				
Si-Si3	-1	7.17609	-8.13623	-3.36944	L				
O-O_2	-1	5.71923	-7.59811	-3.63127	L				
Si-Si3	-1	-7.02662	-8.25406	-3.38337	L				
O-O_2	-1	-5.57838	-7.69184	-3.64235	L				
Si-Si3	-1	-4.46085	0.12678	-4.56589	L				
Si-Si3	-1	-3.63061	-2.51824	-3.30987	L	H-H_	77	0.	0.
Si-Si3	-1	-2.84543	-7.46669	-0.96408	L				
O-O_2	-1	-3.57986	-1.07436	-3.99308	L				
O-O_2	-1	-5.07877	-3.08057	-3.05093	L				
O-O_2	-1	-1.24628	-7.70875	-0.84167	L				
Si-Si3	-1	4.47394	0.20091	-4.55713	L				
Si-Si3	-1	3.6853	-2.45842	-3.303	L	H-H_	73	0.	0.
Si-Si3	-1	2.97767	-7.41838	-0.95837	L				
O-O_2	-1	3.61187	-1.0147	-3.98603	L				
O-O_2	-1	5.14266	-2.99577	-3.0409	L				
O-O_2	-1	1.38316	-7.68694	-0.83909	L				
Si-Si3	-1	6.66094	-3.38066	-2.85129	L				
Si-Si3	-1	8.07424	-5.77528	-1.71101	L				
O-O_2	-1	6.85052	-4.83472	-2.16217	L				
Si-Si3	-1	-6.59083	-3.4906	-2.86429	L				
Si-Si3	-1	-7.96643	-5.90836	-1.72675	L				
O-O_2	-1	-6.75825	-4.94763	-2.17552	L				
Si-Si3	-1	-4.06632	-7.28181	-3.829	L				
Si-Si3	-1	-2.69072	-4.86405	-4.96654	L				
O-O_2	-1	-1.26369	-5.46791	-4.67374	L				
O-O_2	-1	-3.8989	-5.82478	-4.51777	L				
Si-Si3	-1	4.20159	-7.21321	-3.82089	L				
Si-Si3	-1	2.7883	-4.81859	-4.96116	L				
O-O_2	-1	1.37026	-5.44605	-4.67115	L				
O-O_2	-1	4.01136	-5.75915	-4.51001	L				
O-O_2	-1	-5.37908	0.71528	-3.46321	L				
O-O_2	-1	5.38076	0.80455	-3.45266	L				
O-O_2	-1	0.06083	-6.56595	-2.76184	L				
O-O_2	-1	0.0499	-5.49376	-0.49673	H				
O-O_2	-1	8.01471	-5.043	2.09814	L				
O-O_2	-1	7.46032	-1.27516	0.31714	L				
O-O_2	-1	-7.93765	-4.1028	4.34851	L				
O-O_2	-1	-7.44231	-0.33007	2.56038	L				
O-O_2	-1	-2.7752	-1.31074	0.28083	H				
O-O_2	-1	-3.27036	-5.0873	2.06095	L				
O-O_2	0	2.60369	-0.19841	2.58583	H				
O-O_2	-1	3.34664	-3.9577	4.33798	L				

O-O_3	0	2.56865	-1.27566	0.2572	H				
O-O_2	-1	3.35781	-5.03242	2.06747	L				
O-O_2	-1	-2.78598	-0.23993	2.5433	H				
O-O_2	-1	-3.28151	-4.01269	4.33148	L				
O-O_2	-1	-7.92653	-5.17526	2.08251	L				
O-O_2	-1	-7.43123	-1.39868	0.30253	L				
O-O_2	-1	8.00359	-3.97053	4.36414	L				
O-O_2	-1	7.44923	-0.20655	2.575	L				
Si-Si3	-1	0.0397	-4.73893	3.30188	L	H-H_	173	0.	0.
Si-Si3	-1	0.03819	-4.13602	0.24131	H				
Si-Si3	-1	7.15386	-5.99301	1.15894	L				
Si-Si3	-1	7.86199	-1.03229	-1.18542	L				
O-O_2	-1	7.21913	0.2641	-1.80214	L				
O-O_2	-1	5.69701	-5.45492	0.89705	L				
Si-Si3	-1	-7.04884	-6.11085	1.14501	L				
Si-Si3	-1	-7.83394	-1.16251	-1.20082	L				
O-O_2	-1	-7.21147	0.14437	-1.81629	L				
O-O_2	-1	-5.6006	-5.54863	0.88603	L				
Si-Si3	-1	-4.48308	2.27	-0.03751	L				
Si-Si3	-1	-3.65278	-0.37518	1.21837	H				
Si-Si3	-1	-2.86766	-5.32347	3.5643	L				
O-O_2	-1	-3.60206	1.06885	0.53529	L	H-H_	145	0.	0.
O-O_2	-1	-5.10098	-0.9373	1.4776	L	H-H_	145	0.	0.
O-O_2	-1	-1.2685	-5.56554	3.68671	L				
Si-Si3	0	4.43804	2.32388	-0.02118	H				
Si-Si3	-1	2.95545	-5.27516	3.57001	L				
O-O_2	0	3.36782	1.23844	0.38819	H				
O-O_2	0	5.11098	-0.87524	1.42283	H				
O-O_2	-1	1.36094	-5.54372	3.68929	L				
Si-Si3	-1	6.63866	-1.23735	1.67701	L	H-H_	153	0.	0.
Si-Si3	-1	8.05201	-3.63206	2.81737	L				
O-O_2	-1	6.8283	-2.69151	2.36621	L				
Si-Si3	-1	-6.61305	-1.34739	1.66409	L				
Si-Si3	-1	-7.98865	-3.76515	2.80164	L				
O-O_2	-1	-6.78048	-2.80441	2.35286	L				
Si-Si3	-1	-4.08854	-5.1386	0.69939	L				
Si-Si3	-1	-2.71273	-2.72106	-0.43807	H				
O-O_2	-1	-1.25742	-3.30884	-0.14187	H				
O-O_2	-1	-3.92115	-3.68151	0.01065	L	H-H_	162	0.	0.
Si-Si3	-1	4.1791	-5.06956	0.70737	L	H-H_	168	0.	0.
Si-Si3	0	2.81309	-2.74551	-0.46212	H				
O-O_2	0	1.43555	-3.4608	-0.14664	H				
O-O_2	0	4.12449	-3.54639	0.01927	H				
O-O_2	-1	5.36934	1.87611	-1.1884	H				

O-O_2	-1	-5.4013	2.85849	1.06517	L				
O-O_2	-1	-5.39019	1.78689	-1.19902	L				
O-O_2	-1	5.35853	2.94728	1.07564	H				
O-O_2	-1	0.03855	-4.42299	1.76522	H				
O-O_2	-1	0.02749	-3.35069	4.03164	L				
O-O_2	-1	7.43809	0.86809	4.84551	L				
O-O_2	-1	-2.79729	0.8325	4.80936	L				
O-O_2	-1	2.78082	0.87902	4.81414	H				
O-O_2	-1	-7.45345	0.74453	4.83091	L				
Si-Si3	-1	0.01509	-1.95048	4.7545	L	H-H_	204	0.	0.
Si-Si3	-1	7.13164	-3.84979	5.68732	L				
Si-Si3	-1	7.83977	1.11093	3.34296	L				
O-O_2	-1	7.19691	2.40731	2.72624	L				
O-O_2	-1	5.67478	-3.31168	5.42549	L				
Si-Si3	-1	-7.07106	-3.96763	5.67339	L				
Si-Si3	-1	-7.85616	0.98071	3.32756	L				
O-O_2	-1	-7.23369	2.28759	2.71209	L				
O-O_2	-1	-5.62282	-3.40541	5.41441	L				
Si-Si3	-1	-4.5053	4.41322	4.49087	L				
Si-Si3	-1	-3.67497	1.76808	5.74685	L				
O-O_2	-1	-3.62431	3.21207	5.06368	L				
O-O_2	-1	-5.12321	1.20586	6.00583	L				
Si-Si3	-1	4.42949	4.48735	4.49963	L				
Si-Si3	-1	3.64114	1.8286	5.75441	L	H-H_	177	0.	0.
O-O_2	-1	3.56743	3.27174	5.07073	L				
O-O_2	-1	5.09821	1.29067	6.01586	L				
Si-Si3	-1	6.6165	0.90578	6.20547	L				
Si-Si3	-1	-6.63527	0.79583	6.19247	L				
Si-Si3	-1	-4.11077	-2.99538	5.22776	L				
Si-Si3	-1	-2.73516	-0.5776	4.09023	L	H-H_	128	0.	0.
O-O_2	-1	-1.30814	-1.18147	4.38302	L				
O-O_2	-1	-3.94334	-1.53835	4.539	L				
Si-Si3	-1	4.15713	-2.92685	5.23574	L	H-H_	205	0.	0.
Si-Si3	0	2.73348	-0.54653	4.11672	H				
O-O_2	-1	1.32586	-1.16056	4.38434	H				
O-O_2	-1	3.96698	-1.47232	4.54715	H				
O-O_2	-1	5.34742	4.01937	3.33991	L				
O-O_2	-1	-5.41242	3.9301	3.32936	L				
H-H_	-1	-7.07322	-9.58218	-2.75502	L				
H-H_	-1	-7.09545	-7.43897	1.77336	L				
H-H_	-1	-7.11767	-5.29575	6.30174	L				
H-H_	-1	-3.42716	-8.68802	-0.3889	L				
H-H_	-1	-3.44938	-6.54481	4.13948	L				
H-H_	-1	3.57846	-8.6299	-0.38203	L				

H-H_	-1	3.55623	-6.48668	4.14635	L
H-H_	-1	7.22186	-7.32016	1.78739	L
H-H_	-1	7.19963	-5.17694	6.31577	L
H-H_	-1	7.9279	-2.97106	6.55605	L
H-H_	-1	-9.28323	-0.94313	-1.31176	L
H-H_	-1	-7.34758	-3.53805	-4.12364	L
H-H_	-1	-9.29667	-5.34546	-1.99969	L
H-H_	-1	-7.82837	-8.37912	-4.60912	L
H-H_	-1	-7.92938	3.82375	-4.84222	L
H-H_	-1	-7.93965	4.81439	-2.74911	L
H-H_	-1	-5.32064	-0.33112	-5.6668	L
H-H_	-1	-9.30546	1.20009	3.21662	L
H-H_	-1	-9.31889	-3.20225	2.52869	L
H-H_	-1	-7.96188	6.9576	1.77927	L
H-H_	-1	-7.9516	5.96697	-0.31383	L
H-H_	-1	-2.87161	10.79076	-0.00385	L
H-H_	-1	7.24408	-9.46338	-2.74099	L
H-H_	-1	9.39549	-5.19038	-1.98136	L
H-H_	-1	9.37327	-3.04716	2.54702	L
H-H_	-1	9.30764	-0.7888	-1.29357	L
H-H_	-1	9.28542	1.35442	3.23481	L
H-H_	-1	7.84911	7.08859	1.79458	L
H-H_	-1	7.85938	6.09818	-0.29806	L
H-H_	-1	7.87133	4.94538	-2.7338	L
H-H_	-1	7.8816	3.95496	-4.82644	L
H-H_	-1	-2.86129	9.79542	-2.10689	L
H-H_	-1	-2.84939	8.64754	-4.53223	L
H-H_	-1	-2.83907	7.6522	-6.63527	L
H-H_	-1	2.73162	7.69843	-6.62982	L
H-H_	-1	2.7213	8.69378	-4.52676	L
H-H_	-1	2.7094	9.84164	-2.10144	L
H-H_	-1	2.69908	10.83699	0.00162	L
H-H_	-1	-7.40228	1.73677	7.02147	L
H-H_	-1	-5.37562	4.97101	5.53601	L
H-H_	-1	-3.35518	8.1036	4.0477	L
H-H_	-1	-2.87363	1.89347	6.97283	L
H-H_	-1	-0.07276	8.76549	3.75205	L
H-H_	-1	2.83522	1.94081	6.97816	L
H-H_	-1	3.21974	8.15803	4.05407	L
H-H_	-1	5.28878	5.05935	5.54622	L
H-H_	-1	7.36616	1.8593	7.03595	L
H-H_	-1	3.27459	2.86808	-7.123	L
H-H_	-1	5.34376	-0.24253	-5.65607	L
H-H_	-1	7.42085	-3.41552	-4.10916	L

H-H_	-1	7.98262	-8.24791	-4.59334	L
H-H_	-1	2.83263	-4.5045	-6.39653	L
H-H_	-1	3.45193	-8.16674	-4.65137	L
H-H_	-1	0.07111	-7.54378	-4.97697	L
H-H_	-1	-2.73804	-4.55073	-6.40198	L
H-H_	-1	-3.29932	-8.22275	-4.65799	L
H-H_	-1	-7.88308	-3.10205	6.54074	L
H-H_	-1	-6.78717	-0.52604	6.81735	L
H-H_	-1	-3.30033	2.81355	-7.1296	L
H-H_	-1	-0.0179	3.47427	-7.42771	L
H-H_	-1	0.01631	-2.258	6.1913	L
H-H_	-1	3.39724	-2.89192	6.49374	L
H-H_	-1	6.7885	-0.41347	6.83069	L
H-H_	-1	-3.35401	-2.94793	6.48712	L
Al-Al3	0	3.60354	-0.17269	1.26305	H
H-H_	0	0.82754	-0.03611	-0.05714	H
C-C_3	0	0.29723	0.87439	0.22061	H
C-C_3	0	0.24065	1.05393	1.74176	H
H-H_	0	0.80163	1.71956	-0.2571	H
H-H_	0	-0.72053	0.80628	-0.17624	H
C-C_3	0	1.57257	1.26776	2.45241	H
C-C_3	0	-0.5837	2.3131	2.09976	H
H-H_	0	2.17331	2.02098	1.95262	H
H-H_	0	1.38521	1.56696	3.47502	H
H-H_	0	-0.08483	3.22334	1.74402	H
H-H_	0	-1.56455	2.27241	1.62572	H
H-H_	0	-0.74076	2.41374	3.17994	H
H-H_	0	-0.25936	0.18576	2.18155	H

S4. The coordinates for the adsorption of isobutene on HZSM-23

O-O_2	-1	3.29007	3.95874	-4.95187	L			
O-O_2	-1	-3.33808	3.90375	-4.95837	L			
Si-Si3	-1	-0.01685	3.17755	-5.98797	L			
Si-Si3	-1	-2.92423	2.59327	-5.7257	L			
O-O_2	-1	-3.5467	1.28608	-5.11008	L			
O-O_2	-1	-1.32507	2.3509	-5.60314	L			
Si-Si3	-1	2.89888	2.64158	-5.71999	L			
O-O_2	-1	3.54174	1.3449	-5.10313	L			
O-O_2	-1	1.30437	2.37271	-5.60057	L			
O-O_2	-1	-0.02908	4.56604	-5.25836	L			
O-O_2	-1	-3.34916	4.97235	-2.70052	L			
O-O_2	-1	3.26782	6.10194	-0.42344	L	H-H_	28	0. 0.
O-O_2	-1	3.279	5.02741	-2.69401	L	H-H_	28	0. 0.
O-O_2	-1	-3.3603	6.04696	-0.42999	L			

Si-Si3	-1	-0.03907	5.32077	-1.45959	L				
Si-Si3	-1	-0.0414	5.96545	-4.53614	L				
Si-Si3	-1	6.28701	1.40849	-2.34827	L	H-H_	169	0.	0.
Si-Si3	-1	7.07507	4.06664	-3.60254	L				
O-O_2	-1	7.149	2.62369	-2.91924	L				
O-O_2	-1	5.61821	4.60506	-3.86451	L				
Si-Si3	-1	-6.29731	1.30397	-2.36063	L				
Si-Si3	-1	-7.12763	3.9488	-3.61646	L				
O-O_2	-1	-7.1783	2.50482	-2.93329	L				
O-O_2	-1	-5.6794	4.51133	-3.87559	L				
Si-Si3	-1	-2.94645	4.73648	-1.19732	L				
O-O_2	-1	-3.56892	3.4293	-0.5817	L				
O-O_2	-1	-1.34729	4.49412	-1.07476	L				
Si-Si3	-1	2.87671	4.78476	-1.19183	H				
O-O_2	-1	3.51938	3.48793	-0.57413	H				
O-O_2	-1	1.28217	4.51581	-1.0723	L	H-H_	28	0.	0.
Si-Si3	-1	-4.16734	4.92105	-4.06209	L				
Si-Si3	-1	-2.79174	7.33912	-5.19977	L				
O-O_2	-1	-1.36471	6.73526	-4.90697	L				
O-O_2	-1	-3.99992	6.37839	-4.751	L				
Si-Si3	-1	4.10057	4.98965	-4.05398	L				
Si-Si3	-1	2.68728	7.38458	-5.1944	L				
O-O_2	-1	1.26925	6.75711	-4.90439	L				
O-O_2	-1	3.91035	6.44402	-4.74324	L				
O-O_2	-1	-0.04019	5.6368	-2.99598	L				
O-O_2	-1	-0.05131	6.70926	-0.72998	L				
O-O_2	-1	-3.37138	7.11557	1.82786	L				
O-O_2	-1	3.25676	7.17056	1.83436	L				
Si-Si3	-1	-0.06129	7.46399	3.0688	L				
Si-Si3	-1	-0.06362	8.10867	-0.00776	L				
Si-Si3	-1	6.26473	3.55174	2.18	L	H-H_	172	0.	0.
Si-Si3	-1	7.05285	6.20986	0.92585	L				
O-O_2	-1	7.12677	4.7669	1.60914	L				
O-O_2	-1	5.59599	6.74828	0.66387	L				
Si-Si3	-1	-6.31954	3.44719	2.16775	L				
Si-Si3	-1	-7.14986	6.09202	0.91192	L				
O-O_2	-1	-7.20053	4.64803	1.59509	L				
O-O_2	-1	-5.70162	6.65454	0.65279	L				
Si-Si3	-1	-2.96867	6.8797	3.33106	L				
O-O_2	-1	-3.59114	5.57252	3.94668	L				
O-O_2	-1	-1.36951	6.63733	3.45362	L				
Si-Si3	-1	2.85443	6.92801	3.33677	L				
O-O_2	-1	3.4973	5.63133	3.95363	L				
O-O_2	-1	1.25992	6.65915	3.4562	L				

Si-Si3	-1	-4.18956	7.06427	0.46629	L			
Si-Si3	-1	-2.81396	9.48234	-0.67139	L			
O-O_2	-1	-1.38693	8.87848	-0.37859	L			
O-O_2	-1	-4.02214	8.5216	-0.22262	L			
Si-Si3	-1	4.07835	7.13287	0.4744	L			
Si-Si3	-1	2.66505	9.52779	-0.66602	L			
O-O_2	-1	1.24702	8.90033	-0.37601	L			
O-O_2	-1	3.88812	8.58723	-0.21486	L			
O-O_2	-1	-0.06241	7.78001	1.5324	L			
O-O_2	-1	8.03693	-7.18579	-2.42934	L			
O-O_2	-1	-7.91543	-6.24601	-0.17987	L			
O-O_2	-1	-7.42009	-2.47329	-1.968	L			
O-O_2	-1	-2.75283	-3.45437	-4.24831	L			
O-O_2	-1	-3.24814	-7.23051	-2.46743	L			
O-O_2	0	2.81459	-2.33589	-1.97845	H			
O-O_2	-1	3.36893	-6.10098	-0.19039	L			
O-O_2	-1	2.82496	-3.40809	-4.24284	L			
O-O_2	-1	3.38	-7.17552	-2.46093	L			
O-O_2	-1	-2.76395	-2.38333	-1.98509	H			
O-O_2	-1	-3.25929	-6.15591	-0.1969	L			
O-O_2	-1	-7.90431	-7.31805	-2.44497	L			
O-O_2	-1	8.02581	-6.11375	-0.16424	L			
O-O_2	-1	7.47145	-2.34974	-1.9534	L			
Si-Si3	-1	0.06183	-6.88213	-1.22644	L	H-H_	117	0. 0.
Si-Si3	-1	0.05961	-6.23742	-4.30305	L			
Si-Si3	-1	7.17609	-8.13623	-3.36944	L			
O-O_2	-1	5.71923	-7.59811	-3.63127	L			
Si-Si3	-1	-7.02662	-8.25406	-3.38337	L			
O-O_2	-1	-5.57838	-7.69184	-3.64235	L			
Si-Si3	-1	-4.46085	0.12678	-4.56589	L			
Si-Si3	-1	-3.63061	-2.51824	-3.30987	L	H-H_	77	0. 0.
Si-Si3	-1	-2.84543	-7.46669	-0.96408	L			
O-O_2	-1	-3.57986	-1.07436	-3.99308	L			
O-O_2	-1	-5.07877	-3.08057	-3.05093	L			
O-O_2	-1	-1.24628	-7.70875	-0.84167	L			
Si-Si3	-1	4.47394	0.20091	-4.55713	L			
Si-Si3	-1	3.6853	-2.45842	-3.303	L	H-H_	73	0. 0.
Si-Si3	-1	2.97767	-7.41838	-0.95837	L			
O-O_2	-1	3.61187	-1.0147	-3.98603	L			
O-O_2	-1	5.14266	-2.99577	-3.0409	L			
O-O_2	-1	1.38316	-7.68694	-0.83909	L			
Si-Si3	-1	6.66094	-3.38066	-2.85129	L			
Si-Si3	-1	8.07424	-5.77528	-1.71101	L			
O-O_2	-1	6.85052	-4.83472	-2.16217	L			

Si-Si3	-1	-6.59083	-3.4906	-2.86429	L			
Si-Si3	-1	-7.96643	-5.90836	-1.72675	L			
O-O_2	-1	-6.75825	-4.94763	-2.17552	L			
Si-Si3	-1	-4.06632	-7.28181	-3.829	L			
Si-Si3	-1	-2.69072	-4.86405	-4.96654	L			
O-O_2	-1	-1.26369	-5.46791	-4.67374	L			
O-O_2	-1	-3.8989	-5.82478	-4.51777	L			
Si-Si3	-1	4.20159	-7.21321	-3.82089	L			
Si-Si3	-1	2.7883	-4.81859	-4.96116	L			
O-O_2	-1	1.37026	-5.44605	-4.67115	L			
O-O_2	-1	4.01136	-5.75915	-4.51001	L			
O-O_2	-1	-5.37908	0.71528	-3.46321	L			
O-O_2	-1	5.38076	0.80455	-3.45266	L			
O-O_2	-1	0.06083	-6.56595	-2.76184	L			
O-O_2	-1	0.0499	-5.49376	-0.49673	H			
O-O_2	-1	8.01471	-5.043	2.09814	L			
O-O_2	-1	7.46032	-1.27516	0.31714	L			
O-O_2	-1	-7.93765	-4.1028	4.34851	L			
O-O_2	-1	-7.44231	-0.33007	2.56038	L			
O-O_2	-1	-2.7752	-1.31074	0.28083	H			
O-O_2	-1	-3.27036	-5.0873	2.06095	L			
O-O_2	0	2.60369	-0.19841	2.58583	H			
O-O_2	-1	3.34664	-3.9577	4.33798	L			
O-O_3	0	2.56865	-1.27566	0.2572	H			
O-O_2	-1	3.35781	-5.03242	2.06747	L			
O-O_2	-1	-2.78598	-0.23993	2.5433	H			
O-O_2	-1	-3.28151	-4.01269	4.33148	L			
O-O_2	-1	-7.92653	-5.17526	2.08251	L			
O-O_2	-1	-7.43123	-1.39868	0.30253	L			
O-O_2	-1	8.00359	-3.97053	4.36414	L			
O-O_2	-1	7.44923	-0.20655	2.575	L			
Si-Si3	-1	0.0397	-4.73893	3.30188	L	H-H_	173	0. 0.
Si-Si3	-1	0.03819	-4.13602	0.24131	H			
Si-Si3	-1	7.15386	-5.99301	1.15894	L			
Si-Si3	-1	7.86199	-1.03229	-1.18542	L			
O-O_2	-1	7.21913	0.2641	-1.80214	L			
O-O_2	-1	5.69701	-5.45492	0.89705	L			
Si-Si3	-1	-7.04884	-6.11085	1.14501	L			
Si-Si3	-1	-7.83394	-1.16251	-1.20082	L			
O-O_2	-1	-7.21147	0.14437	-1.81629	L			
O-O_2	-1	-5.6006	-5.54863	0.88603	L			
Si-Si3	-1	-4.48308	2.27	-0.03751	L			
Si-Si3	-1	-3.65278	-0.37518	1.21837	H			
Si-Si3	-1	-2.86766	-5.32347	3.5643	L			

O-O_2	-1	-3.60206	1.06885	0.53529	L	H-H_	145	0.	0.
O-O_2	-1	-5.10098	-0.9373	1.4776	L	H-H_	145	0.	0.
O-O_2	-1	-1.2685	-5.56554	3.68671	L				
Si-Si3	0	4.43804	2.32388	-0.02118	H				
Si-Si3	-1	2.95545	-5.27516	3.57001	L				
O-O_2	0	3.36782	1.23844	0.38819	H				
O-O_2	0	5.11098	-0.87524	1.42283	H				
O-O_2	-1	1.36094	-5.54372	3.68929	L				
Si-Si3	-1	6.63866	-1.23735	1.67701	L	H-H_	153	0.	0.
Si-Si3	-1	8.05201	-3.63206	2.81737	L				
O-O_2	-1	6.8283	-2.69151	2.36621	L				
Si-Si3	-1	-6.61305	-1.34739	1.66409	L				
Si-Si3	-1	-7.98865	-3.76515	2.80164	L				
O-O_2	-1	-6.78048	-2.80441	2.35286	L				
Si-Si3	-1	-4.08854	-5.1386	0.69939	L				
Si-Si3	-1	-2.71273	-2.72106	-0.43807	H				
O-O_2	-1	-1.25742	-3.30884	-0.14187	H				
O-O_2	-1	-3.92115	-3.68151	0.01065	L	H-H_	162	0.	0.
Si-Si3	-1	4.1791	-5.06956	0.70737	L	H-H_	168	0.	0.
Si-Si3	0	2.81309	-2.74551	-0.46212	H				
O-O_2	0	1.43555	-3.4608	-0.14664	H				
O-O_2	0	4.12449	-3.54639	0.01927	H				
O-O_2	-1	5.36934	1.87611	-1.1884	H				
O-O_2	-1	-5.4013	2.85849	1.06517	L				
O-O_2	-1	-5.39019	1.78689	-1.19902	L				
O-O_2	-1	5.35853	2.94728	1.07564	H				
O-O_2	-1	0.03855	-4.42299	1.76522	H				
O-O_2	-1	0.02749	-3.35069	4.03164	L				
O-O_2	-1	7.43809	0.86809	4.84551	L				
O-O_2	-1	-2.79729	0.8325	4.80936	L				
O-O_2	-1	2.78082	0.87902	4.81414	H				
O-O_2	-1	-7.45345	0.74453	4.83091	L				
Si-Si3	-1	0.01509	-1.95048	4.7545	L	H-H_	204	0.	0.
Si-Si3	-1	7.13164	-3.84979	5.68732	L				
Si-Si3	-1	7.83977	1.11093	3.34296	L				
O-O_2	-1	7.19691	2.40731	2.72624	L				
O-O_2	-1	5.67478	-3.31168	5.42549	L				
Si-Si3	-1	-7.07106	-3.96763	5.67339	L				
Si-Si3	-1	-7.85616	0.98071	3.32756	L				
O-O_2	-1	-7.23369	2.28759	2.71209	L				
O-O_2	-1	-5.62282	-3.40541	5.41441	L				
Si-Si3	-1	-4.5053	4.41322	4.49087	L				
Si-Si3	-1	-3.67497	1.76808	5.74685	L				
O-O_2	-1	-3.62431	3.21207	5.06368	L				

O-O_2	-1	-5.12321	1.20586	6.00583	L			
Si-Si3	-1	4.42949	4.48735	4.49963	L			
Si-Si3	-1	3.64114	1.8286	5.75441	L	H-H_	177	0. 0.
O-O_2	-1	3.56743	3.27174	5.07073	L			
O-O_2	-1	5.09821	1.29067	6.01586	L			
Si-Si3	-1	6.6165	0.90578	6.20547	L			
Si-Si3	-1	-6.63527	0.79583	6.19247	L			
Si-Si3	-1	-4.11077	-2.99538	5.22776	L			
Si-Si3	-1	-2.73516	-0.5776	4.09023	L	H-H_	128	0. 0.
O-O_2	-1	-1.30814	-1.18147	4.38302	L			
O-O_2	-1	-3.94334	-1.53835	4.539	L			
Si-Si3	-1	4.15713	-2.92685	5.23574	L	H-H_	205	0. 0.
Si-Si3	0	2.73348	-0.54653	4.11672	H			
O-O_2	-1	1.32586	-1.16056	4.38434	H			
O-O_2	-1	3.96698	-1.47232	4.54715	H			
O-O_2	-1	5.34742	4.01937	3.33991	L			
O-O_2	-1	-5.41242	3.9301	3.32936	L			
H-H_	-1	-7.07322	-9.58218	-2.75502	L			
H-H_	-1	-7.09545	-7.43897	1.77336	L			
H-H_	-1	-7.11767	-5.29575	6.30174	L			
H-H_	-1	-3.42716	-8.68802	-0.3889	L			
H-H_	-1	-3.44938	-6.54481	4.13948	L			
H-H_	-1	3.57846	-8.6299	-0.38203	L			
H-H_	-1	3.55623	-6.48668	4.14635	L			
H-H_	-1	7.22186	-7.32016	1.78739	L			
H-H_	-1	7.19963	-5.17694	6.31577	L			
H-H_	-1	7.9279	-2.97106	6.55605	L			
H-H_	-1	-9.28323	-0.94313	-1.31176	L			
H-H_	-1	-7.34758	-3.53805	-4.12364	L			
H-H_	-1	-9.29667	-5.34546	-1.99969	L			
H-H_	-1	-7.82837	-8.37912	-4.60912	L			
H-H_	-1	-7.92938	3.82375	-4.84222	L			
H-H_	-1	-7.93965	4.81439	-2.74911	L			
H-H_	-1	-5.32064	-0.33112	-5.6668	L			
H-H_	-1	-9.30546	1.20009	3.21662	L			
H-H_	-1	-9.31889	-3.20225	2.52869	L			
H-H_	-1	-7.96188	6.9576	1.77927	L			
H-H_	-1	-7.9516	5.96697	-0.31383	L			
H-H_	-1	-2.87161	10.79076	-0.00385	L			
H-H_	-1	7.24408	-9.46338	-2.74099	L			
H-H_	-1	9.39549	-5.19038	-1.98136	L			
H-H_	-1	9.37327	-3.04716	2.54702	L			
H-H_	-1	9.30764	-0.7888	-1.29357	L			
H-H_	-1	9.28542	1.35442	3.23481	L			

H-H_	-1	7.84911	7.08859	1.79458	L
H-H_	-1	7.85938	6.09818	-0.29806	L
H-H_	-1	7.87133	4.94538	-2.7338	L
H-H_	-1	7.8816	3.95496	-4.82644	L
H-H_	-1	-2.86129	9.79542	-2.10689	L
H-H_	-1	-2.84939	8.64754	-4.53223	L
H-H_	-1	-2.83907	7.6522	-6.63527	L
H-H_	-1	2.73162	7.69843	-6.62982	L
H-H_	-1	2.7213	8.69378	-4.52676	L
H-H_	-1	2.7094	9.84164	-2.10144	L
H-H_	-1	2.69908	10.83699	0.00162	L
H-H_	-1	-7.40228	1.73677	7.02147	L
H-H_	-1	-5.37562	4.97101	5.53601	L
H-H_	-1	-3.35518	8.1036	4.0477	L
H-H_	-1	-2.87363	1.89347	6.97283	L
H-H_	-1	-0.07276	8.76549	3.75205	L
H-H_	-1	2.83522	1.94081	6.97816	L
H-H_	-1	3.21974	8.15803	4.05407	L
H-H_	-1	5.28878	5.05935	5.54622	L
H-H_	-1	7.36616	1.8593	7.03595	L
H-H_	-1	3.27459	2.86808	-7.123	L
H-H_	-1	5.34376	-0.24253	-5.65607	L
H-H_	-1	7.42085	-3.41552	-4.10916	L
H-H_	-1	7.98262	-8.24791	-4.59334	L
H-H_	-1	2.83263	-4.5045	-6.39653	L
H-H_	-1	3.45193	-8.16674	-4.65137	L
H-H_	-1	0.07111	-7.54378	-4.97697	L
H-H_	-1	-2.73804	-4.55073	-6.40198	L
H-H_	-1	-3.29932	-8.22275	-4.65799	L
H-H_	-1	-7.88308	-3.10205	6.54074	L
H-H_	-1	-6.78717	-0.52604	6.81735	L
H-H_	-1	-3.30033	2.81355	-7.1296	L
H-H_	-1	-0.0179	3.47427	-7.42771	L
H-H_	-1	0.01631	-2.258	6.1913	L
H-H_	-1	3.39724	-2.89192	6.49374	L
H-H_	-1	6.7885	-0.41347	6.83069	L
H-H_	-1	-3.35401	-2.94793	6.48712	L
Al-Al3	0	3.60354	-0.17269	1.26305	H
H-H_	0	0.95233	1.2425	-0.05728	H
C-C_3	0	0.0207	1.59759	0.38454	H
C-C_2	0	0.238	2.17158	1.75592	H
H-H_	0	-0.40374	2.3628	-0.27487	H
H-H_	0	-0.69857	0.7732	0.41112	H
C-C_2	0	1.473	2.33487	2.26746	H

C-C_3	0	-0.944	2.68236	2.52525	H
H-H_	0	2.32668	2.28233	1.60354	H
H-H_	0	1.60781	2.79133	3.24255	H
H-H_	0	-1.19169	3.67996	2.13498	H
H-H_	0	-1.8308	2.06191	2.41201	H
H-H_	0	-0.70694	2.80022	3.58649	H
H-H_	0	1.95769	0.53796	2.37055	H

S5. The coordinates for the adsorption of 1-butene on HZSM-48

O-O_2	-1	-5.97438	-1.97428	-3.89564	L
O-O_2	-1	-3.45925	-2.50664	-4.44428	L
O-O_2	-1	-5.95227	-6.30455	-3.795	L
Si-Si3	-1	-4.4501	-1.54024	-3.62311	L
Si-Si3	-1	-4.56516	-6.30018	-4.61452	L
O-O_2	-1	-1.34412	3.87136	-4.44159	L
Si-Si3	-1	-2.73122	3.86699	-3.62207	L
O-O_2	-1	-5.99217	1.90059	-4.34181	L
O-O_2	-1	-3.48085	2.45546	-3.79801	L
Si-Si3	-1	-4.46458	1.48022	-4.61728	L
O-O_2	-1	-1.28674	-8.23402	-3.88601	L
O-O_2	-1	-3.80292	-7.70413	-4.43225	L
O-O_2	-1	-1.30868	-3.90334	-3.80484	L
Si-Si3	-1	-2.8105	-8.66682	-3.60863	L
Si-Si3	-1	-2.69735	-3.9114	-4.62168	L
O-O_2	-1	-8.6133	1.88886	-4.33928	L
O-O_2	-1	3.43326	2.48643	-3.80468	L
Si-Si3	-1	-10.13803	1.45481	-4.61181	L
O-O_2	-1	1.33439	-8.22228	-3.88854	L
O-O_2	-1	1.31813	-3.89158	-3.80737	L
Si-Si3	-1	2.86294	-8.64141	-3.6141	L
Si-Si3	-1	2.70524	-3.88721	-4.62689	L
O-O_2	-1	-8.59552	-1.98602	-3.89312	L
O-O_2	-1	3.45486	-2.47567	-4.45095	L
Si-Si3	-1	-10.12354	-1.56565	-3.61765	L
O-O_2	-1	1.2827	3.88313	-4.44413	L
Si-Si3	-1	2.67137	3.89119	-3.62728	L
O-O_2	-1	-7.27586	-4.15485	-4.56896	L
Si-Si3	-1	-7.26926	-5.41041	-3.56118	L
Si-Si3	-1	-7.28313	-2.54615	-4.63772	L
Si-Si3	-1	-0.03518	4.77682	-4.67946	L
O-O_2	-1	-7.31183	4.07003	-3.66597	L
Si-Si3	-1	-7.30455	2.46133	-3.5972	L
O-O_2	-1	0.01344	-6.05652	-4.57163	L
Si-Si3	-1	0.00876	-4.79642	-3.5695	L H-H_ 95 0. 0.

Si-Si3	-1	0.02059	-7.66551	-4.63316	L			
O-O_2	-1	-4.21401	-0.02892	-4.12043	L			
O-O_2	-1	-10.37367	-0.05651	-4.11449	L			
O-O_2	-1	-3.63074	-5.10456	-4.07413	L			
O-O_2	-1	1.31195	3.84986	0.29242	L			
Si-Si3	-1	2.71188	3.88772	-0.55504	L			
O-O_2	-1	-5.96651	-1.95569	4.3615	L			
O-O_2	-1	-3.45137	-2.48804	3.81286	L			
O-O_R	-1	-5.9444	-6.28595	4.46189	L			
Si-Si3	-1	-4.44222	-1.52164	4.63402	L			
Si-Si3	-1	-4.55729	-6.28158	3.64237	L			
O-O_2	-1	-1.33624	3.88996	3.8153	L			
Si-Si3	-1	-2.72335	3.88559	4.63507	L			
O-O_2	-1	-8.592	-1.97771	-0.20225	L			
O-O_3	0	3.46162	-2.29756	0.46943	H			
Si-Si3	-1	-10.12054	-1.55858	-0.47669	L			
O-O_2	-1	-5.98429	1.91919	3.91508	L			
O-O_2	-1	-3.47297	2.47406	4.45888	L			
Si-Si3	-1	-4.45671	1.49882	3.63961	L			
O-O_2	-1	1.33791	-8.21397	-0.19767	L			
O-O_2	0	1.2117	-3.78211	-0.47028	H			
Si-Si3	-1	2.86594	-8.63434	-0.47314	L			
O-O_2	-1	-8.60894	1.89914	0.22674	L			
O-O_2	-1	3.43377	2.44825	-0.37569	L	H-H_	163	0. 0.
Si-Si3	-1	-10.13314	1.46633	0.50413	L			
O-O_2	-1	-1.27887	-8.21542	4.37113	L			
O-O_2	-1	-3.79505	-7.68553	3.82489	L			
O-O_2	-1	-1.3008	-3.88474	4.45206	L			
Si-Si3	-1	-2.80263	-8.64822	4.64852	L			
Si-Si3	-1	-2.68947	-3.8928	3.6352	L			
O-O_2	-1	-8.60542	1.90745	3.91761	L			
O-O_2	-1	3.44114	2.50502	4.45221	L			
Si-Si3	-1	-10.13015	1.47341	3.64508	L			
O-O_2	-1	-1.28322	-8.2257	-0.19515	L			
O-O_2	-1	-3.79836	-7.69335	0.35349	L			
O-O_2	0	-1.40144	-3.86134	-0.36014	H			
Si-Si3	-1	-2.80751	-8.65975	-0.46767	L			
Si-Si3	-1	-2.74963	-3.91773	0.56113	H			
O-O_2	-1	-5.98781	1.91088	0.22422	L			
O-O_2	-1	-3.47754	2.46328	-0.32687	L			
Si-Si3	-1	-4.481	1.48075	0.50002	L			
O-O_2	-1	1.34227	-8.20368	4.3686	L			
O-O_2	-1	1.32601	-3.87298	4.44952	L	H-H_	80	0. 0.
Si-Si3	-1	2.87081	-8.62282	4.64305	L			

Si-Si3	0	2.71312	-3.8686	3.63001	H			
O-O_2	-1	-1.34468	3.84345	0.28372	L			
Si-Si3	-1	-2.75707	3.87568	-0.5464	L			
O-O_2	-1	-8.58764	-1.96743	4.36402	L			
O-O_2	-1	3.46274	-2.45707	3.80619	L	H-H_	80	0. 0.
Si-Si3	-1	-10.11566	-1.54705	4.63949	L			
O-O_2	-1	1.29057	3.90173	3.81277	L			
Si-Si3	-1	2.67924	3.90979	4.62986	L			
O-O_2	-1	-6.08416	-1.8723	-0.39229	L			
O-O_2	-1	-3.60323	-2.51667	0.48651	L	H-H_	73	0. 0.
O-O_R	-1	-5.94892	-6.29664	-0.2857	L			
Si-Si3	-1	-4.50172	-1.5615	-0.49395	L			
Si-Si3	-1	-4.56025	-6.28859	0.53114	L			
O-O_R	-1	-7.2702	-4.87436	-2.04235	L			
O-O_2	-1	-7.30961	4.80814	2.06439	L			
O-O_2	-1	-0.03782	-5.5026	-2.06961	H			
O-O_2	-1	-7.27885	-2.05567	2.07983	L			
O-O_2	-1	-7.30096	1.98945	-2.05778	L			
O-O_2	-1	0.02913	-8.12572	2.08653	L			
O-O_2	-1	-3.98872	-1.7521	-2.03159	L			
O-O_2	-1	-10.45046	-1.6812	-2.04651	L			
O-O_2	-1	-4.12978	1.61498	2.06855	L			
O-O_2	-1	3.19286	-8.51879	-2.04412	L			
O-O_2	-1	-10.46113	1.58662	2.07466	L			
O-O_2	-1	-3.13849	-8.54714	-2.03801	L			
O-O_2	-1	2.34844	4.14737	-2.07184	L			
O-O_2	-1	-4.88318	-6.03302	2.0865	L			
O-O_2	-1	-2.40761	4.12607	-2.06726	L			
O-O_2	0	2.22866	-4.14452	2.13262	H			
O-O_2	-1	-2.24564	-4.21334	2.07366	L	H-H_	73	0. 0.
Si-Si3	-1	-0.0258	4.76756	0.55282	L			
O-O_R	-1	-7.26798	-4.13625	3.68793	L			
Si-	-1	-7.26139	-5.39181	4.69572	L			
Si-Si3	-1	-7.27526	-2.52755	3.61917	L			
Si-Si3	-1	-0.02731	4.79542	3.57768	L			
O-O_R	-1	-7.27104	-4.14347	0.48109	L			
Si-	-1	-7.26637	-5.40356	-0.52104	L			
Si-Si3	-1	-7.27819	-2.53447	0.54262	L			
O-O_2	-1	-7.30395	4.08863	4.59093	L			
Si-Si3	-1	-7.29668	2.47993	4.65994	L			
O-O_2	-1	0.00666	-5.98223	0.54898	H			
Si-Si3	0	-0.04282	-4.79033	-0.60047	H			
Si-Si3	-1	0.02553	-7.65383	0.54718	L	H-H_	120	0. 0.
O-O_2	-1	-7.30877	4.07725	-0.45888	L			

Si-Si3	-1	-7.30162	2.46826	-0.52065	L			
O-O_2	-1	0.02132	-6.03792	3.68526	L			
Si-Si3	-1	0.01664	-4.77783	4.68739	L			
Si-Si3	-1	0.02846	-7.64691	3.62373	L			
O-O_2	-1	-4.20613	-0.01032	4.13646	L			
O-O_2	-1	-10.36974	-0.04721	0.01408	L			
O-O_2	-1	-10.3658	-0.03791	4.1424	L			
O-O_2	-1	-4.22151	-0.03194	-0.01742	L			
O-O_2	-1	-3.62286	-5.08597	4.18301	L			
O-O_2	-1	-3.64994	-5.08836	-0.13674	L	H-H_	73	0. 0.
O-O_2	-1	8.58732	-1.90907	-3.90968	L			
Si-Si3	-1	10.11161	-1.47502	-3.63715	L			
O-O_2	-1	8.56953	1.96581	-4.35585	L			
Si-Si3	-1	10.09712	1.54544	-4.63132	L			
O-O_2	-1	5.9484	1.95407	-4.35332	L			
Si-Si3	-1	4.42411	1.52003	-4.62585	L			
O-O_2	-1	3.8451	-7.66988	-4.43962	L			
O-O_2	-1	5.96619	-1.92081	-3.90715	L			
O-O_2	-1	5.98262	-6.2511	-3.8065	L			
Si-Si3	-1	4.43861	-1.50043	-3.63171	L	H-H_	180	0. 0.
Si-Si3	-1	4.59438	-6.25915	-4.62335	L			
O-O_2	-1	7.28584	-4.08963	-4.583	L			
Si-Si3	-1	7.29244	-5.34519	-3.57521	L			
Si-Si3	-1	7.27857	-2.48093	-4.65176	L			
O-O_2	-1	7.24988	4.13525	-3.68	L			
Si-Si3	-1	7.25715	2.52654	-3.61124	L			
O-O_2	-1	10.34769	0.0363	-4.13447	L			
O-O_2	-1	4.18803	0.00871	-4.12853	L			
O-O_2	-1	3.65019	-5.07195	-4.08115	L			
O-O_2	-1	8.5952	-1.89047	4.34746	L			
Si-Si3	-1	10.11948	-1.45642	4.61999	L			
O-O_2	-1	6.06404	-1.85361	-0.39998	H			
O-O_2	-1	5.98597	-6.24319	-0.29721	L			
Si-Si3	0	4.52093	-1.46397	-0.54527	H			
Si-Si3	-1	4.59928	-6.24755	0.52231	L	H-H_	198	0. 0.
O-O_2	-1	8.57741	1.98441	3.90105	L			
Si-Si3	-1	10.105	1.56403	3.62558	L			
O-O_2	-1	3.84967	-7.6591	0.34612	L			
O-O_2	-1	5.95276	1.96431	0.21271	L	H-H_	163	0. 0.
Si-Si3	-1	4.45654	1.54611	0.49373	H			
O-O_2	-1	5.95628	1.97267	3.90357	L			
Si-Si3	-1	4.43199	1.53863	3.63105	L			
O-O_2	-1	8.57389	1.9761	0.21018	L			
Si-Si3	-1	10.102	1.55696	0.48462	L			

O-O_2	-1	3.85298	-7.65128	3.81752	L			
O-O_2	-1	5.97406	-1.90221	4.34999	L			
O-O_2	-1	5.9905	-6.2325	4.45039	L			
Si-Si3	-1	4.44648	-1.48183	4.62546	L			
Si-Si3	-1	4.60226	-6.24056	3.63354	L			
O-O_2	-1	8.59084	-1.90075	-0.21881	L			
Si-Si3	-1	10.1146	-1.46795	-0.4962	L			
O-O_2	-1	7.2915	-4.80914	-2.05638	L			
O-O_2	-1	7.25209	4.87336	2.05036	L			
O-O_2	-1	7.28285	-1.99045	2.06579	L			
O-O_2	-1	7.26075	2.05467	-2.07181	L			
O-O_2	-1	10.44302	-1.58763	-2.06665	L			
O-O_2	-1	3.98214	-1.71211	-2.04598	H			
O-O_2	-1	10.43236	1.6802	2.05452	L			
O-O_2	-1	4.10057	1.65185	2.06063	L	H-H_	163	0. 0.
O-O_2	-1	4.92292	-5.9891	2.07705	L			
O-O_2	-1	7.29372	-4.07103	3.6739	L			
Si-Si3	-1	7.30031	-5.3266	4.68168	L			
Si-Si3	-1	7.28645	-2.46233	3.60513	L			
O-O_2	-1	7.29066	-4.07826	0.46705	L			
Si-Si3	-1	7.29534	-5.33835	-0.53508	L			
Si-Si3	-1	7.28351	-2.46926	0.52858	L	H-H_	155	0. 0.
O-O_2	-1	7.25775	4.15385	4.57689	L			
Si-Si3	-1	7.26502	2.54514	4.6459	L			
O-O_2	-1	7.25293	4.14247	-0.47291	L			
Si-Si3	-1	7.26007	2.5335	-0.53469	L			
O-O_2	-1	10.35557	0.0549	4.12242	L			
O-O_2	0	4.24006	0.0359	-0.04362	H			
O-O_2	-1	4.1959	0.02731	4.12836	L			
O-O_2	-1	10.35163	0.0456	-0.0059	L			
O-O_2	0	3.75852	-5.0662	-0.16924	H			
O-O_2	-1	3.65806	-5.05336	4.17599	L	H-H_	80	0. 0.
O-O_2	-1	-1.36081	8.20267	-4.36042	L			
O-O_2	-1	-3.87109	7.65028	-3.80934	L			
Si-Si3	-1	-2.88892	8.62181	-4.63487	L			
O-O_2	-1	-6.00904	6.2315	-4.44246	L			
Si-Si3	-1	-4.62037	6.23955	-3.62561	L			
O-O_2	-1	1.26032	8.21442	-4.36295	L			
Si-Si3	-1	2.78452	8.64722	-4.64034	L			
O-O_2	-1	-0.03986	6.0363	-3.67733	L			
Si-Si3	-1	-0.04701	7.6453	-3.6158	L			
Si-Si3	-1	-7.31842	5.32498	-4.67375	L			
O-O_2	-1	-3.67632	5.05215	-4.16781	L			
O-O_2	-1	1.26468	8.2247	0.20308	L			

Si-Si3	-1	2.7894	8.65874	0.4756	L
O-O_2	-1	-1.35294	8.22127	3.89647	L
O-O_2	-1	-3.86322	7.66887	4.44755	L
Si-Si3	-1	-2.88105	8.64041	3.62203	L
O-O_2	-1	-6.00117	6.25009	3.81443	L
Si-Si3	-1	-4.61249	6.25815	4.63153	L
O-O_2	-1	-6.00451	6.24219	0.30539	L
Si-Si3	-1	-4.6174	6.24656	-0.51439	L
O-O_2	-1	-1.35646	8.21296	0.2056	L
O-O_2	-1	-3.86778	7.65809	-0.33819	L
Si-Si3	-1	-2.88404	8.63333	0.48107	L
O-O_2	-1	1.2682	8.23301	3.89394	L
Si-Si3	-1	2.7924	8.66582	3.61656	L
O-O_2	-1	-0.03114	5.32401	2.05629	L
O-O_2	-1	-0.04767	8.1241	-2.07851	L
O-O_2	-1	3.12038	8.54614	2.04603	L
O-O_2	-1	-3.21097	8.51778	2.05213	L
O-O_2	-1	-4.94102	5.98748	-2.06903	L
O-O_2	-1	-0.0368	6.04353	-0.47024	L
Si-Si3	-1	-0.04407	7.65223	-0.53925	L
O-O_2	-1	-0.03198	6.0549	4.57956	L
Si-Si3	-1	-0.03913	7.6639	4.64134	L
Si-Si3	-1	-7.31054	5.34358	3.58339	L
Si-Si3	-1	-7.31344	5.33673	0.54301	L
O-O_2	-1	-3.66844	5.07075	4.08908	L
O-O_2	-1	-3.67231	5.06161	0.0316	L
O-O_2	-1	5.92585	6.28495	-4.45396	L
Si-Si3	-1	4.53918	6.28057	-3.63444	L
O-O_2	-1	3.77694	7.68453	-3.81672	L
Si-Si3	-1	7.24328	5.3902	-4.68779	L
O-O_2	-1	3.60461	5.08476	-4.17483	L
O-O_2	-1	3.78025	7.69235	-0.34557	L
O-O_2	-1	5.93038	6.29564	0.29388	L
Si-Si3	-1	4.54214	6.28758	-0.52322	L
O-O_2	-1	5.93373	6.30354	3.80293	L
Si-Si3	-1	4.54705	6.29917	4.6227	L
O-O_2	-1	3.78481	7.70312	4.44018	L
O-O_2	-1	4.86507	6.0314	-2.07849	L
Si-Si3	-1	7.25116	5.4088	3.56935	L
Si-Si3	-1	7.24826	5.40195	0.52897	L
O-O_2	-1	3.60861	5.09422	0.02458	L
O-O_2	-1	3.61248	5.10336	4.08206	L
H-H_	-1	-3.08969	9.83732	-4.24037	L
H-H_	-1	-3.08556	9.84706	0.08148	L

H-H_	-1	-3.08181	9.85592	4.01652	L
H-H_	-1	2.9748	9.86453	-4.2462	L
H-H_	-1	2.97892	9.87427	0.07562	L
H-H_	-1	2.98268	9.88313	4.0107	L
H-H_	-1	8.29594	6.11874	-4.50191	L
H-H_	-1	8.30058	6.12965	0.338	L
H-H_	-1	8.30384	6.13735	3.75504	L
H-H_	-1	10.88785	2.32933	-3.97279	L
H-H_	-1	10.89147	2.33788	-0.17893	L
H-H_	-1	10.89572	2.34793	4.2841	L
H-H_	-1	10.3603	1.63883	-5.89441	L
H-H_	-1	-8.3772	6.04406	-4.48583	L
H-H_	-1	-8.37261	6.05498	0.35407	L
H-H_	-1	-8.36935	6.06268	3.77111	L
H-H_	-1	-10.93447	2.2316	-3.95176	L
H-H_	-1	-10.93085	2.24014	-0.1579	L
H-H_	-1	-10.92659	2.2502	4.30514	L
H-H_	-1	-10.37854	-1.63996	5.90269	L
H-H_	-1	-10.90639	-2.33095	3.98097	L
H-H_	-1	-10.91001	-2.3395	0.18687	L
H-H_	-1	-10.91427	-2.34955	-4.27617	L
H-H_	-1	-8.32215	-6.13861	-3.7471	L
H-H_	-1	10.90805	-2.25181	-4.29721	L
H-H_	-1	10.91231	-2.24176	0.16583	L
H-H_	-1	10.91593	-2.23321	3.95994	L
H-H_	-1	10.38595	-1.54696	5.8826	L
H-H_	-1	8.35144	-6.06393	-3.76317	L
H-H_	-1	8.3547	-6.05624	-0.3459	L
H-H_	-1	8.35931	-6.04534	4.49372	L
H-H_	-1	3.07123	-9.83832	4.24835	L
H-H_	-1	3.1361	-8.52421	5.90531	L
H-H_	-1	-2.99325	-9.86543	4.25421	L
H-H_	-1	-3.06635	-8.55199	5.91129	L
H-H_	-1	-2.99737	-9.87516	-0.06753	L
H-H_	-1	-3.00113	-9.88409	-4.00275	L
H-H_	-1	3.0671	-9.84805	-0.07336	L
H-H_	-1	3.06336	-9.85698	-4.00861	L
H-H_	-1	4.85218	-6.05699	-5.87478	L
H-H_	-1	7.27568	-2.10182	-5.88856	L
H-H_	-1	0.02112	-8.05019	-5.86824	L
H-H_	-1	2.44506	-4.095	-5.8769	L
H-H_	-1	7.24403	4.9601	-5.9078	L
H-H_	-1	4.15768	1.61105	-5.88844	L
H-H_	-1	-2.43773	-4.11687	-5.87219	L

H-H_	-1	-4.82717	-6.10034	-5.86545	L
H-H_	-1	3.04821	8.551	-5.90311	L
H-H_	-1	-0.03826	5.20141	-5.90139	L
H-H_	-1	-7.28602	-2.16703	-5.87452	L
H-H_	-1	-4.20174	1.57361	-5.88045	L
H-H_	-1	-3.15418	8.52322	-5.89714	L
H-H_	-1	-7.31767	4.89489	-5.89376	L
H-H_	-1	-10.40413	1.54583	-5.87447	L
H-H_	-1	-7.29379	2.10078	5.89672	L
H-H_	-1	-4.8703	6.05549	5.88287	L
H-H_	-1	-0.03966	8.04861	5.87641	L
H-H_	-1	-2.46316	4.09389	5.885	L
H-H_	-1	-7.26214	-4.9613	5.91558	L
H-H_	-1	-4.17609	-1.61219	5.89671	L
H-H_	-1	2.41961	4.11576	5.88029	L
H-H_	-1	4.80907	6.09884	5.87354	L
H-H_	-1	0.01972	-5.20284	5.90918	L
H-H_	-1	4.18326	-1.57474	5.88858	L
H-H_	-1	7.26791	2.16599	5.88269	L
H-H_	-1	7.29956	-4.89609	5.90154	L
C-C_2	0	1.17251	-0.46314	1.75475	H
C-C_2	0	0.63891	-0.83768	0.58119	H
H-H_	0	1.64137	0.50802	1.89365	H
H-H_	0	1.10476	-1.11129	2.62508	H
H-H_	0	0.17483	-1.81896	0.50431	H
C-C_3	0	0.65258	-0.03349	-0.69063	H
C-C_3	0	-0.73017	0.04111	-1.35979	H
H-H_	0	1.34772	-0.52126	-1.38936	H
H-H_	0	1.04082	0.97186	-0.49781	H
H-H_	0	-0.66556	0.58526	-2.30906	H
H-H_	0	-1.12487	-0.95818	-1.56912	H
H-H_	0	-1.45433	0.56243	-0.72909	H
Al-Al3	0	2.62114	-4.02325	0.50948	H
H-H_	0	2.78936	-1.66805	0.84284	H

S6. The coordinates for INT1 on HZSM-48

O-O_2	-1	-5.97438	-1.97428	-3.89564	L
O-O_2	-1	-3.45925	-2.50664	-4.44428	L
O-O_2	-1	-5.95227	-6.30455	-3.795	L
Si-Si3	-1	-4.4501	-1.54024	-3.62311	L
Si-Si3	-1	-4.56516	-6.30018	-4.61452	L
O-O_2	-1	-1.34412	3.87136	-4.44159	L
Si-Si3	-1	-2.73122	3.86699	-3.62207	L
O-O_2	-1	-5.99217	1.90059	-4.34181	L

O-O_2	-1	-3.48085	2.45546	-3.79801	L			
Si-Si3	-1	-4.46458	1.48022	-4.61728	L			
O-O_2	-1	-1.28674	-8.23402	-3.88601	L			
O-O_2	-1	-3.80292	-7.70413	-4.43225	L			
O-O_2	-1	-1.30868	-3.90334	-3.80484	L			
Si-Si3	-1	-2.8105	-8.66682	-3.60863	L			
Si-Si3	-1	-2.69735	-3.9114	-4.62168	L			
O-O_2	-1	-8.6133	1.88886	-4.33928	L			
O-O_2	-1	3.43326	2.48643	-3.80468	L			
Si-Si3	-1	-10.13803	1.45481	-4.61181	L			
O-O_2	-1	1.33439	-8.22228	-3.88854	L			
O-O_2	-1	1.31813	-3.89158	-3.80737	L			
Si-Si3	-1	2.86294	-8.64141	-3.6141	L			
Si-Si3	-1	2.70524	-3.88721	-4.62689	L			
O-O_2	-1	-8.59552	-1.98602	-3.89312	L			
O-O_2	-1	3.45486	-2.47567	-4.45095	L			
Si-Si3	-1	-10.12354	-1.56565	-3.61765	L			
O-O_2	-1	1.2827	3.88313	-4.44413	L			
Si-Si3	-1	2.67137	3.89119	-3.62728	L			
O-O_2	-1	-7.27586	-4.15485	-4.56896	L			
Si-Si3	-1	-7.26926	-5.41041	-3.56118	L			
Si-Si3	-1	-7.28313	-2.54615	-4.63772	L			
Si-Si3	-1	-0.03518	4.77682	-4.67946	L			
O-O_2	-1	-7.31183	4.07003	-3.66597	L			
Si-Si3	-1	-7.30455	2.46133	-3.5972	L			
O-O_2	-1	0.01344	-6.05652	-4.57163	L			
Si-Si3	-1	0.00876	-4.79642	-3.5695	L	H-H_	95	0. 0.
Si-Si3	-1	0.02059	-7.66551	-4.63316	L			
O-O_2	-1	-4.21401	-0.02892	-4.12043	L			
O-O_2	-1	-10.37367	-0.05651	-4.11449	L			
O-O_2	-1	-3.63074	-5.10456	-4.07413	L			
O-O_2	-1	1.31195	3.84986	0.29242	L			
Si-Si3	-1	2.71188	3.88772	-0.55504	L			
O-O_2	-1	-5.96651	-1.95569	4.3615	L			
O-O_2	-1	-3.45137	-2.48804	3.81286	L			
O-O_R	-1	-5.9444	-6.28595	4.46189	L			
Si-Si3	-1	-4.44222	-1.52164	4.63402	L			
Si-Si3	-1	-4.55729	-6.28158	3.64237	L			
O-O_2	-1	-1.33624	3.88996	3.8153	L			
Si-Si3	-1	-2.72335	3.88559	4.63507	L			
O-O_2	-1	-8.592	-1.97771	-0.20225	L			
O-O_3	0	3.46162	-2.29756	0.46943	H			
Si-Si3	-1	-10.12054	-1.55858	-0.47669	L			
O-O_2	-1	-5.98429	1.91919	3.91508	L			

O-O_2	-1	-3.47297	2.47406	4.45888	L			
Si-Si3	-1	-4.45671	1.49882	3.63961	L			
O-O_2	-1	1.33791	-8.21397	-0.19767	L			
O-O_2	0	1.2117	-3.78211	-0.47028	H			
Si-Si3	-1	2.86594	-8.63434	-0.47314	L			
O-O_2	-1	-8.60894	1.89914	0.22674	L			
O-O_2	-1	3.43377	2.44825	-0.37569	L	H-H_	163	0. 0.
Si-Si3	-1	-10.13314	1.46633	0.50413	L			
O-O_2	-1	-1.27887	-8.21542	4.37113	L			
O-O_2	-1	-3.79505	-7.68553	3.82489	L			
O-O_2	-1	-1.3008	-3.88474	4.45206	L			
Si-Si3	-1	-2.80263	-8.64822	4.64852	L			
Si-Si3	-1	-2.68947	-3.8928	3.6352	L			
O-O_2	-1	-8.60542	1.90745	3.91761	L			
O-O_2	-1	3.44114	2.50502	4.45221	L			
Si-Si3	-1	-10.13015	1.47341	3.64508	L			
O-O_2	-1	-1.28322	-8.2257	-0.19515	L			
O-O_2	-1	-3.79836	-7.69335	0.35349	L			
O-O_2	0	-1.40144	-3.86134	-0.36014	H			
Si-Si3	-1	-2.80751	-8.65975	-0.46767	L			
Si-Si3	-1	-2.74963	-3.91773	0.56113	H			
O-O_2	-1	-5.98781	1.91088	0.22422	L			
O-O_2	-1	-3.47754	2.46328	-0.32687	L			
Si-Si3	-1	-4.481	1.48075	0.50002	L			
O-O_2	-1	1.34227	-8.20368	4.3686	L			
O-O_2	-1	1.32601	-3.87298	4.44952	L	H-H_	80	0. 0.
Si-Si3	-1	2.87081	-8.62282	4.64305	L			
Si-Si3	0	2.71312	-3.8686	3.63001	H			
O-O_2	-1	-1.34468	3.84345	0.28372	L			
Si-Si3	-1	-2.75707	3.87568	-0.5464	L			
O-O_2	-1	-8.58764	-1.96743	4.36402	L			
O-O_2	-1	3.46274	-2.45707	3.80619	L	H-H_	80	0. 0.
Si-Si3	-1	-10.11566	-1.54705	4.63949	L			
O-O_2	-1	1.29057	3.90173	3.81277	L			
Si-Si3	-1	2.67924	3.90979	4.62986	L			
O-O_2	-1	-6.08416	-1.8723	-0.39229	L			
O-O_2	-1	-3.60323	-2.51667	0.48651	L	H-H_	73	0. 0.
O-O_R	-1	-5.94892	-6.29664	-0.2857	L			
Si-Si3	-1	-4.50172	-1.5615	-0.49395	L			
Si-Si3	-1	-4.56025	-6.28859	0.53114	L			
O-O_R	-1	-7.2702	-4.87436	-2.04235	L			
O-O_2	-1	-7.30961	4.80814	2.06439	L			
O-O_2	-1	-0.03782	-5.5026	-2.06961	H			
O-O_2	-1	-7.27885	-2.05567	2.07983	L			

O-O_2	-1	-7.30096	1.98945	-2.05778	L			
O-O_2	-1	0.02913	-8.12572	2.08653	L			
O-O_2	-1	-3.98872	-1.7521	-2.03159	L			
O-O_2	-1	-10.45046	-1.6812	-2.04651	L			
O-O_2	-1	-4.12978	1.61498	2.06855	L			
O-O_2	-1	3.19286	-8.51879	-2.04412	L			
O-O_2	-1	-10.46113	1.58662	2.07466	L			
O-O_2	-1	-3.13849	-8.54714	-2.03801	L			
O-O_2	-1	2.34844	4.14737	-2.07184	L			
O-O_2	-1	-4.88318	-6.03302	2.0865	L			
O-O_2	-1	-2.40761	4.12607	-2.06726	L			
O-O_2	0	2.22866	-4.14452	2.13262	H			
O-O_2	-1	-2.24564	-4.21334	2.07366	L	H-H_	73	0. 0.
Si-Si3	-1	-0.0258	4.76756	0.55282	L			
O-O_R	-1	-7.26798	-4.13625	3.68793	L			
Si-	-1	-7.26139	-5.39181	4.69572	L			
Si-Si3	-1	-7.27526	-2.52755	3.61917	L			
Si-Si3	-1	-0.02731	4.79542	3.57768	L			
O-O_R	-1	-7.27104	-4.14347	0.48109	L			
Si-	-1	-7.26637	-5.40356	-0.52104	L			
Si-Si3	-1	-7.27819	-2.53447	0.54262	L			
O-O_2	-1	-7.30395	4.08863	4.59093	L			
Si-Si3	-1	-7.29668	2.47993	4.65994	L			
O-O_2	-1	0.00666	-5.98223	0.54898	H			
Si-Si3	0	-0.04282	-4.79033	-0.60047	H			
Si-Si3	-1	0.02553	-7.65383	0.54718	L	H-H_	120	0. 0.
O-O_2	-1	-7.30877	4.07725	-0.45888	L			
Si-Si3	-1	-7.30162	2.46826	-0.52065	L			
O-O_2	-1	0.02132	-6.03792	3.68526	L			
Si-Si3	-1	0.01664	-4.77783	4.68739	L			
Si-Si3	-1	0.02846	-7.64691	3.62373	L			
O-O_2	-1	-4.20613	-0.01032	4.13646	L			
O-O_2	-1	-10.36974	-0.04721	0.01408	L			
O-O_2	-1	-10.3658	-0.03791	4.1424	L			
O-O_2	-1	-4.22151	-0.03194	-0.01742	L			
O-O_2	-1	-3.62286	-5.08597	4.18301	L			
O-O_2	-1	-3.64994	-5.08836	-0.13674	L	H-H_	73	0. 0.
O-O_2	-1	8.58732	-1.90907	-3.90968	L			
Si-Si3	-1	10.11161	-1.47502	-3.63715	L			
O-O_2	-1	8.56953	1.96581	-4.35585	L			
Si-Si3	-1	10.09712	1.54544	-4.63132	L			
O-O_2	-1	5.9484	1.95407	-4.35332	L			
Si-Si3	-1	4.42411	1.52003	-4.62585	L			
O-O_2	-1	3.8451	-7.66988	-4.43962	L			

O-O_2	-1	5.96619	-1.92081	-3.90715	L				
O-O_2	-1	5.98262	-6.2511	-3.8065	L				
Si-Si3	-1	4.43861	-1.50043	-3.63171	L	H-H_	180	0.	0.
Si-Si3	-1	4.59438	-6.25915	-4.62335	L				
O-O_2	-1	7.28584	-4.08963	-4.583	L				
Si-Si3	-1	7.29244	-5.34519	-3.57521	L				
Si-Si3	-1	7.27857	-2.48093	-4.65176	L				
O-O_2	-1	7.24988	4.13525	-3.68	L				
Si-Si3	-1	7.25715	2.52654	-3.61124	L				
O-O_2	-1	10.34769	0.0363	-4.13447	L				
O-O_2	-1	4.18803	0.00871	-4.12853	L				
O-O_2	-1	3.65019	-5.07195	-4.08115	L				
O-O_2	-1	8.5952	-1.89047	4.34746	L				
Si-Si3	-1	10.11948	-1.45642	4.61999	L				
O-O_2	-1	6.06404	-1.85361	-0.39998	H				
O-O_2	-1	5.98597	-6.24319	-0.29721	L				
Si-Si3	0	4.52093	-1.46397	-0.54527	H				
Si-Si3	-1	4.59928	-6.24755	0.52231	L	H-H_	198	0.	0.
O-O_2	-1	8.57741	1.98441	3.90105	L				
Si-Si3	-1	10.105	1.56403	3.62558	L				
O-O_2	-1	3.84967	-7.6591	0.34612	L				
O-O_2	-1	5.95276	1.96431	0.21271	L	H-H_	163	0.	0.
Si-Si3	-1	4.45654	1.54611	0.49373	H				
O-O_2	-1	5.95628	1.97267	3.90357	L				
Si-Si3	-1	4.43199	1.53863	3.63105	L				
O-O_2	-1	8.57389	1.9761	0.21018	L				
Si-Si3	-1	10.102	1.55696	0.48462	L				
O-O_2	-1	3.85298	-7.65128	3.81752	L				
O-O_2	-1	5.97406	-1.90221	4.34999	L				
O-O_2	-1	5.9905	-6.2325	4.45039	L				
Si-Si3	-1	4.44648	-1.48183	4.62546	L				
Si-Si3	-1	4.60226	-6.24056	3.63354	L				
O-O_2	-1	8.59084	-1.90075	-0.21881	L				
Si-Si3	-1	10.1146	-1.46795	-0.4962	L				
O-O_2	-1	7.2915	-4.80914	-2.05638	L				
O-O_2	-1	7.25209	4.87336	2.05036	L				
O-O_2	-1	7.28285	-1.99045	2.06579	L				
O-O_2	-1	7.26075	2.05467	-2.07181	L				
O-O_2	-1	10.44302	-1.58763	-2.06665	L				
O-O_2	-1	3.98214	-1.71211	-2.04598	H				
O-O_2	-1	10.43236	1.6802	2.05452	L				
O-O_2	-1	4.10057	1.65185	2.06063	L	H-H_	163	0.	0.
O-O_2	-1	4.92292	-5.9891	2.07705	L				
O-O_2	-1	7.29372	-4.07103	3.6739	L				

Si-Si3	-1	7.30031	-5.3266	4.68168	L				
Si-Si3	-1	7.28645	-2.46233	3.60513	L				
O-O_2	-1	7.29066	-4.07826	0.46705	L				
Si-Si3	-1	7.29534	-5.33835	-0.53508	L				
Si-Si3	-1	7.28351	-2.46926	0.52858	L	H-H_	155	0.	0.
O-O_2	-1	7.25775	4.15385	4.57689	L				
Si-Si3	-1	7.26502	2.54514	4.6459	L				
O-O_2	-1	7.25293	4.14247	-0.47291	L				
Si-Si3	-1	7.26007	2.5335	-0.53469	L				
O-O_2	-1	10.35557	0.0549	4.12242	L				
O-O_2	0	4.24006	0.0359	-0.04362	H				
O-O_2	-1	4.1959	0.02731	4.12836	L				
O-O_2	-1	10.35163	0.0456	-0.0059	L				
O-O_2	0	3.75852	-5.0662	-0.16924	H				
O-O_2	-1	3.65806	-5.05336	4.17599	L	H-H_	80	0.	0.
O-O_2	-1	-1.36081	8.20267	-4.36042	L				
O-O_2	-1	-3.87109	7.65028	-3.80934	L				
Si-Si3	-1	-2.88892	8.62181	-4.63487	L				
O-O_2	-1	-6.00904	6.2315	-4.44246	L				
Si-Si3	-1	-4.62037	6.23955	-3.62561	L				
O-O_2	-1	1.26032	8.21442	-4.36295	L				
Si-Si3	-1	2.78452	8.64722	-4.64034	L				
O-O_2	-1	-0.03986	6.0363	-3.67733	L				
Si-Si3	-1	-0.04701	7.6453	-3.6158	L				
Si-Si3	-1	-7.31842	5.32498	-4.67375	L				
O-O_2	-1	-3.67632	5.05215	-4.16781	L				
O-O_2	-1	1.26468	8.2247	0.20308	L				
Si-Si3	-1	2.7894	8.65874	0.4756	L				
O-O_2	-1	-1.35294	8.22127	3.89647	L				
O-O_2	-1	-3.86322	7.66887	4.44755	L				
Si-Si3	-1	-2.88105	8.64041	3.62203	L				
O-O_2	-1	-6.00117	6.25009	3.81443	L				
Si-Si3	-1	-4.61249	6.25815	4.63153	L				
O-O_2	-1	-6.00451	6.24219	0.30539	L				
Si-Si3	-1	-4.6174	6.24656	-0.51439	L				
O-O_2	-1	-1.35646	8.21296	0.2056	L				
O-O_2	-1	-3.86778	7.65809	-0.33819	L				
Si-Si3	-1	-2.88404	8.63333	0.48107	L				
O-O_2	-1	1.2682	8.23301	3.89394	L				
Si-Si3	-1	2.7924	8.66582	3.61656	L				
O-O_2	-1	-0.03114	5.32401	2.05629	L				
O-O_2	-1	-0.04767	8.1241	-2.07851	L				
O-O_2	-1	3.12038	8.54614	2.04603	L				
O-O_2	-1	-3.21097	8.51778	2.05213	L				

O-O_2	-1	-4.94102	5.98748	-2.06903	L
O-O_2	-1	-0.0368	6.04353	-0.47024	L
Si-Si3	-1	-0.04407	7.65223	-0.53925	L
O-O_2	-1	-0.03198	6.0549	4.57956	L
Si-Si3	-1	-0.03913	7.6639	4.64134	L
Si-Si3	-1	-7.31054	5.34358	3.58339	L
Si-Si3	-1	-7.31344	5.33673	0.54301	L
O-O_2	-1	-3.66844	5.07075	4.08908	L
O-O_2	-1	-3.67231	5.06161	0.0316	L
O-O_2	-1	5.92585	6.28495	-4.45396	L
Si-Si3	-1	4.53918	6.28057	-3.63444	L
O-O_2	-1	3.77694	7.68453	-3.81672	L
Si-Si3	-1	7.24328	5.3902	-4.68779	L
O-O_2	-1	3.60461	5.08476	-4.17483	L
O-O_2	-1	3.78025	7.69235	-0.34557	L
O-O_2	-1	5.93038	6.29564	0.29388	L
Si-Si3	-1	4.54214	6.28758	-0.52322	L
O-O_2	-1	5.93373	6.30354	3.80293	L
Si-Si3	-1	4.54705	6.29917	4.6227	L
O-O_2	-1	3.78481	7.70312	4.44018	L
O-O_2	-1	4.86507	6.0314	-2.07849	L
Si-Si3	-1	7.25116	5.4088	3.56935	L
Si-Si3	-1	7.24826	5.40195	0.52897	L
O-O_2	-1	3.60861	5.09422	0.02458	L
O-O_2	-1	3.61248	5.10336	4.08206	L
H-H_	-1	-3.08969	9.83732	-4.24037	L
H-H_	-1	-3.08556	9.84706	0.08148	L
H-H_	-1	-3.08181	9.85592	4.01652	L
H-H_	-1	2.9748	9.86453	-4.2462	L
H-H_	-1	2.97892	9.87427	0.07562	L
H-H_	-1	2.98268	9.88313	4.0107	L
H-H_	-1	8.29594	6.11874	-4.50191	L
H-H_	-1	8.30058	6.12965	0.338	L
H-H_	-1	8.30384	6.13735	3.75504	L
H-H_	-1	10.88785	2.32933	-3.97279	L
H-H_	-1	10.89147	2.33788	-0.17893	L
H-H_	-1	10.89572	2.34793	4.2841	L
H-H_	-1	10.3603	1.63883	-5.89441	L
H-H_	-1	-8.3772	6.04406	-4.48583	L
H-H_	-1	-8.37261	6.05498	0.35407	L
H-H_	-1	-8.36935	6.06268	3.77111	L
H-H_	-1	-10.93447	2.2316	-3.95176	L
H-H_	-1	-10.93085	2.24014	-0.1579	L
H-H_	-1	-10.92659	2.2502	4.30514	L

H-H_	-1	-10.37854	-1.63996	5.90269	L
H-H_	-1	-10.90639	-2.33095	3.98097	L
H-H_	-1	-10.91001	-2.3395	0.18687	L
H-H_	-1	-10.91427	-2.34955	-4.27617	L
H-H_	-1	-8.32215	-6.13861	-3.7471	L
H-H_	-1	10.90805	-2.25181	-4.29721	L
H-H_	-1	10.91231	-2.24176	0.16583	L
H-H_	-1	10.91593	-2.23321	3.95994	L
H-H_	-1	10.38595	-1.54696	5.8826	L
H-H_	-1	8.35144	-6.06393	-3.76317	L
H-H_	-1	8.3547	-6.05624	-0.3459	L
H-H_	-1	8.35931	-6.04534	4.49372	L
H-H_	-1	3.07123	-9.83832	4.24835	L
H-H_	-1	3.1361	-8.52421	5.90531	L
H-H_	-1	-2.99325	-9.86543	4.25421	L
H-H_	-1	-3.06635	-8.55199	5.91129	L
H-H_	-1	-2.99737	-9.87516	-0.06753	L
H-H_	-1	-3.00113	-9.88409	-4.00275	L
H-H_	-1	3.0671	-9.84805	-0.07336	L
H-H_	-1	3.06336	-9.85698	-4.00861	L
H-H_	-1	4.85218	-6.05699	-5.87478	L
H-H_	-1	7.27568	-2.10182	-5.88856	L
H-H_	-1	0.02112	-8.05019	-5.86824	L
H-H_	-1	2.44506	-4.095	-5.8769	L
H-H_	-1	7.24403	4.9601	-5.9078	L
H-H_	-1	4.15768	1.61105	-5.88844	L
H-H_	-1	-2.43773	-4.11687	-5.87219	L
H-H_	-1	-4.82717	-6.10034	-5.86545	L
H-H_	-1	3.04821	8.551	-5.90311	L
H-H_	-1	-0.03826	5.20141	-5.90139	L
H-H_	-1	-7.28602	-2.16703	-5.87452	L
H-H_	-1	-4.20174	1.57361	-5.88045	L
H-H_	-1	-3.15418	8.52322	-5.89714	L
H-H_	-1	-7.31767	4.89489	-5.89376	L
H-H_	-1	-10.40413	1.54583	-5.87447	L
H-H_	-1	-7.29379	2.10078	5.89672	L
H-H_	-1	-4.8703	6.05549	5.88287	L
H-H_	-1	-0.03966	8.04861	5.87641	L
H-H_	-1	-2.46316	4.09389	5.885	L
H-H_	-1	-7.26214	-4.9613	5.91558	L
H-H_	-1	-4.17609	-1.61219	5.89671	L
H-H_	-1	2.41961	4.11576	5.88029	L
H-H_	-1	4.80907	6.09884	5.87354	L
H-H_	-1	0.01972	-5.20284	5.90918	L

H-H_	-1	4.18326	-1.57474	5.88858	L
H-H_	-1	7.26791	2.16599	5.88269	L
H-H_	-1	7.29956	-4.89609	5.90154	L
Al-Al3	0	2.62114	-4.02325	0.50948	H
H-H_	0	-1.04385	-1.74668	0.89336	H
C-C_3	0	0.03439	-1.75508	1.04879	H
C-C_3	0	0.81615	-2.08038	-0.21987	H
H-H_	0	0.33182	-0.75647	1.38408	H
H-H_	0	0.29306	-2.46398	1.83797	H
H-H_	0	1.81427	-1.67133	-0.10678	H
C-C_3	0	0.24865	-1.55221	-1.53134	H
C-C_3	0	0.16262	-0.01664	-1.51927	H
H-H_	0	-0.74015	-1.97689	-1.72859	H
H-H_	0	0.9331	-1.85123	-2.33059	H
H-H_	0	-0.1468	0.34762	-2.50413	H
H-H_	0	-0.56803	0.34934	-0.7924	H
H-H_	0	1.13239	0.43531	-1.28487	H

S7. The coordinates for INT2 on HZSM-48

O-O_2	-1	-5.97438	-1.97428	-3.89564	L
O-O_2	-1	-3.45925	-2.50664	-4.44428	L
O-O_2	-1	-5.95227	-6.30455	-3.795	L
Si-Si3	-1	-4.4501	-1.54024	-3.62311	L
Si-Si3	-1	-4.56516	-6.30018	-4.61452	L
O-O_2	-1	-1.34412	3.87136	-4.44159	L
Si-Si3	-1	-2.73122	3.86699	-3.62207	L
O-O_2	-1	-5.99217	1.90059	-4.34181	L
O-O_2	-1	-3.48085	2.45546	-3.79801	L
Si-Si3	-1	-4.46458	1.48022	-4.61728	L
O-O_2	-1	-1.28674	-8.23402	-3.88601	L
O-O_2	-1	-3.80292	-7.70413	-4.43225	L
O-O_2	-1	-1.30868	-3.90334	-3.80484	L
Si-Si3	-1	-2.8105	-8.66682	-3.60863	L
Si-Si3	-1	-2.69735	-3.9114	-4.62168	L
O-O_2	-1	-8.6133	1.88886	-4.33928	L
O-O_2	-1	3.43326	2.48643	-3.80468	L
Si-Si3	-1	-10.13803	1.45481	-4.61181	L
O-O_2	-1	1.33439	-8.22228	-3.88854	L
O-O_2	-1	1.31813	-3.89158	-3.80737	L
Si-Si3	-1	2.86294	-8.64141	-3.6141	L
Si-Si3	-1	2.70524	-3.88721	-4.62689	L
O-O_2	-1	-8.59552	-1.98602	-3.89312	L
O-O_2	-1	3.45486	-2.47567	-4.45095	L
Si-Si3	-1	-10.12354	-1.56565	-3.61765	L

O-O_2 -1 1.2827 3.88313 -4.44413 L
Si-Si3 -1 2.67137 3.89119 -3.62728 L
O-O_2 -1 -7.27586 -4.15485 -4.56896 L
Si-Si3 -1 -7.26926 -5.41041 -3.56118 L
Si-Si3 -1 -7.28313 -2.54615 -4.63772 L
Si-Si3 -1 -0.03518 4.77682 -4.67946 L
O-O_2 -1 -7.31183 4.07003 -3.66597 L
Si-Si3 -1 -7.30455 2.46133 -3.5972 L
O-O_2 -1 0.01344 -6.05652 -4.57163 L
Si-Si3 -1 0.00876 -4.79642 -3.5695 L H-H_ 95 0. 0.
Si-Si3 -1 0.02059 -7.66551 -4.63316 L
O-O_2 -1 -4.21401 -0.02892 -4.12043 L
O-O_2 -1 -10.37367 -0.05651 -4.11449 L
O-O_2 -1 -3.63074 -5.10456 -4.07413 L
O-O_2 -1 1.31195 3.84986 0.29242 L
Si-Si3 -1 2.71188 3.88772 -0.55504 L
O-O_2 -1 -5.96651 -1.95569 4.3615 L
O-O_2 -1 -3.45137 -2.48804 3.81286 L
O-O_R -1 -5.9444 -6.28595 4.46189 L
Si-Si3 -1 -4.44222 -1.52164 4.63402 L
Si-Si3 -1 -4.55729 -6.28158 3.64237 L
O-O_2 -1 -1.33624 3.88996 3.8153 L
Si-Si3 -1 -2.72335 3.88559 4.63507 L
O-O_2 -1 -8.592 -1.97771 -0.20225 L
O-O_3 0 3.46162 -2.29756 0.46943 H
Si-Si3 -1 -10.12054 -1.55858 -0.47669 L
O-O_2 -1 -5.98429 1.91919 3.91508 L
O-O_2 -1 -3.47297 2.47406 4.45888 L
Si-Si3 -1 -4.45671 1.49882 3.63961 L
O-O_2 -1 1.33791 -8.21397 -0.19767 L
O-O_2 0 1.2117 -3.78211 -0.47028 H
Si-Si3 -1 2.86594 -8.63434 -0.47314 L
O-O_2 -1 -8.60894 1.89914 0.22674 L
O-O_2 -1 3.43377 2.44825 -0.37569 L H-H_ 163 0. 0.
Si-Si3 -1 -10.13314 1.46633 0.50413 L
O-O_2 -1 -1.27887 -8.21542 4.37113 L
O-O_2 -1 -3.79505 -7.68553 3.82489 L
O-O_2 -1 -1.3008 -3.88474 4.45206 L
Si-Si3 -1 -2.80263 -8.64822 4.64852 L
Si-Si3 -1 -2.68947 -3.8928 3.6352 L
O-O_2 -1 -8.60542 1.90745 3.91761 L
O-O_2 -1 3.44114 2.50502 4.45221 L
Si-Si3 -1 -10.13015 1.47341 3.64508 L
O-O_2 -1 -1.28322 -8.2257 -0.19515 L

O-O_2	-1	-3.79836	-7.69335	0.35349	L			
O-O_2	0	-1.40144	-3.86134	-0.36014	H			
Si-Si3	-1	-2.80751	-8.65975	-0.46767	L			
Si-Si3	-1	-2.74963	-3.91773	0.56113	H			
O-O_2	-1	-5.98781	1.91088	0.22422	L			
O-O_2	-1	-3.47754	2.46328	-0.32687	L			
Si-Si3	-1	-4.481	1.48075	0.50002	L			
O-O_2	-1	1.34227	-8.20368	4.3686	L			
O-O_2	-1	1.32601	-3.87298	4.44952	L	H-H_	80	0. 0.
Si-Si3	-1	2.87081	-8.62282	4.64305	L			
Si-Si3	0	2.71312	-3.8686	3.63001	H			
O-O_2	-1	-1.34468	3.84345	0.28372	L			
Si-Si3	-1	-2.75707	3.87568	-0.5464	L			
O-O_2	-1	-8.58764	-1.96743	4.36402	L			
O-O_2	-1	3.46274	-2.45707	3.80619	L	H-H_	80	0. 0.
Si-Si3	-1	-10.11566	-1.54705	4.63949	L			
O-O_2	-1	1.29057	3.90173	3.81277	L			
Si-Si3	-1	2.67924	3.90979	4.62986	L			
O-O_2	-1	-6.08416	-1.8723	-0.39229	L			
O-O_2	-1	-3.60323	-2.51667	0.48651	L	H-H_	73	0. 0.
O-O_R	-1	-5.94892	-6.29664	-0.2857	L			
Si-Si3	-1	-4.50172	-1.5615	-0.49395	L			
Si-Si3	-1	-4.56025	-6.28859	0.53114	L			
O-O_R	-1	-7.2702	-4.87436	-2.04235	L			
O-O_2	-1	-7.30961	4.80814	2.06439	L			
O-O_2	-1	-0.03782	-5.5026	-2.06961	H			
O-O_2	-1	-7.27885	-2.05567	2.07983	L			
O-O_2	-1	-7.30096	1.98945	-2.05778	L			
O-O_2	-1	0.02913	-8.12572	2.08653	L			
O-O_2	-1	-3.98872	-1.7521	-2.03159	L			
O-O_2	-1	-10.45046	-1.6812	-2.04651	L			
O-O_2	-1	-4.12978	1.61498	2.06855	L			
O-O_2	-1	3.19286	-8.51879	-2.04412	L			
O-O_2	-1	-10.46113	1.58662	2.07466	L			
O-O_2	-1	-3.13849	-8.54714	-2.03801	L			
O-O_2	-1	2.34844	4.14737	-2.07184	L			
O-O_2	-1	-4.88318	-6.03302	2.0865	L			
O-O_2	-1	-2.40761	4.12607	-2.06726	L			
O-O_2	0	2.22866	-4.14452	2.13262	H			
O-O_2	-1	-2.24564	-4.21334	2.07366	L	H-H_	73	0. 0.
Si-Si3	-1	-0.0258	4.76756	0.55282	L			
O-O_R	-1	-7.26798	-4.13625	3.68793	L			
Si-	-1	-7.26139	-5.39181	4.69572	L			
Si-Si3	-1	-7.27526	-2.52755	3.61917	L			

Si-Si3	-1	-0.02731	4.79542	3.57768	L			
O-O_R	-1	-7.27104	-4.14347	0.48109	L			
Si-	-1	-7.26637	-5.40356	-0.52104	L			
Si-Si3	-1	-7.27819	-2.53447	0.54262	L			
O-O_2	-1	-7.30395	4.08863	4.59093	L			
Si-Si3	-1	-7.29668	2.47993	4.65994	L			
O-O_2	-1	0.00666	-5.98223	0.54898	H			
Si-Si3	0	-0.04282	-4.79033	-0.60047	H			
Si-Si3	-1	0.02553	-7.65383	0.54718	L	H-H_	120	0. 0.
O-O_2	-1	-7.30877	4.07725	-0.45888	L			
Si-Si3	-1	-7.30162	2.46826	-0.52065	L			
O-O_2	-1	0.02132	-6.03792	3.68526	L			
Si-Si3	-1	0.01664	-4.77783	4.68739	L			
Si-Si3	-1	0.02846	-7.64691	3.62373	L			
O-O_2	-1	-4.20613	-0.01032	4.13646	L			
O-O_2	-1	-10.36974	-0.04721	0.01408	L			
O-O_2	-1	-10.3658	-0.03791	4.1424	L			
O-O_2	-1	-4.22151	-0.03194	-0.01742	L			
O-O_2	-1	-3.62286	-5.08597	4.18301	L			
O-O_2	-1	-3.64994	-5.08836	-0.13674	L	H-H_	73	0. 0.
O-O_2	-1	8.58732	-1.90907	-3.90968	L			
Si-Si3	-1	10.11161	-1.47502	-3.63715	L			
O-O_2	-1	8.56953	1.96581	-4.35585	L			
Si-Si3	-1	10.09712	1.54544	-4.63132	L			
O-O_2	-1	5.9484	1.95407	-4.35332	L			
Si-Si3	-1	4.42411	1.52003	-4.62585	L			
O-O_2	-1	3.8451	-7.66988	-4.43962	L			
O-O_2	-1	5.96619	-1.92081	-3.90715	L			
O-O_2	-1	5.98262	-6.2511	-3.8065	L			
Si-Si3	-1	4.43861	-1.50043	-3.63171	L	H-H_	180	0. 0.
Si-Si3	-1	4.59438	-6.25915	-4.62335	L			
O-O_2	-1	7.28584	-4.08963	-4.583	L			
Si-Si3	-1	7.29244	-5.34519	-3.57521	L			
Si-Si3	-1	7.27857	-2.48093	-4.65176	L			
O-O_2	-1	7.24988	4.13525	-3.68	L			
Si-Si3	-1	7.25715	2.52654	-3.61124	L			
O-O_2	-1	10.34769	0.0363	-4.13447	L			
O-O_2	-1	4.18803	0.00871	-4.12853	L			
O-O_2	-1	3.65019	-5.07195	-4.08115	L			
O-O_2	-1	8.5952	-1.89047	4.34746	L			
Si-Si3	-1	10.11948	-1.45642	4.61999	L			
O-O_2	-1	6.06404	-1.85361	-0.39998	H			
O-O_2	-1	5.98597	-6.24319	-0.29721	L			
Si-Si3	0	4.52093	-1.46397	-0.54527	H			

Si-Si3	-1	4.59928	-6.24755	0.52231	L	H-H_	198	0.	0.
O-O_2	-1	8.57741	1.98441	3.90105	L				
Si-Si3	-1	10.105	1.56403	3.62558	L				
O-O_2	-1	3.84967	-7.6591	0.34612	L				
O-O_2	-1	5.95276	1.96431	0.21271	L	H-H_	163	0.	0.
Si-Si3	-1	4.45654	1.54611	0.49373	H				
O-O_2	-1	5.95628	1.97267	3.90357	L				
Si-Si3	-1	4.43199	1.53863	3.63105	L				
O-O_2	-1	8.57389	1.9761	0.21018	L				
Si-Si3	-1	10.102	1.55696	0.48462	L				
O-O_2	-1	3.85298	-7.65128	3.81752	L				
O-O_2	-1	5.97406	-1.90221	4.34999	L				
O-O_2	-1	5.9905	-6.2325	4.45039	L				
Si-Si3	-1	4.44648	-1.48183	4.62546	L				
Si-Si3	-1	4.60226	-6.24056	3.63354	L				
O-O_2	-1	8.59084	-1.90075	-0.21881	L				
Si-Si3	-1	10.1146	-1.46795	-0.4962	L				
O-O_2	-1	7.2915	-4.80914	-2.05638	L				
O-O_2	-1	7.25209	4.87336	2.05036	L				
O-O_2	-1	7.28285	-1.99045	2.06579	L				
O-O_2	-1	7.26075	2.05467	-2.07181	L				
O-O_2	-1	10.44302	-1.58763	-2.06665	L				
O-O_2	-1	3.98214	-1.71211	-2.04598	H				
O-O_2	-1	10.43236	1.6802	2.05452	L				
O-O_2	-1	4.10057	1.65185	2.06063	L	H-H_	163	0.	0.
O-O_2	-1	4.92292	-5.9891	2.07705	L				
O-O_2	-1	7.29372	-4.07103	3.6739	L				
Si-Si3	-1	7.30031	-5.3266	4.68168	L				
Si-Si3	-1	7.28645	-2.46233	3.60513	L				
O-O_2	-1	7.29066	-4.07826	0.46705	L				
Si-Si3	-1	7.29534	-5.33835	-0.53508	L				
Si-Si3	-1	7.28351	-2.46926	0.52858	L	H-H_	155	0.	0.
O-O_2	-1	7.25775	4.15385	4.57689	L				
Si-Si3	-1	7.26502	2.54514	4.6459	L				
O-O_2	-1	7.25293	4.14247	-0.47291	L				
Si-Si3	-1	7.26007	2.5335	-0.53469	L				
O-O_2	-1	10.35557	0.0549	4.12242	L				
O-O_2	0	4.24006	0.0359	-0.04362	H				
O-O_2	-1	4.1959	0.02731	4.12836	L				
O-O_2	-1	10.35163	0.0456	-0.0059	L				
O-O_2	0	3.75852	-5.0662	-0.16924	H				
O-O_2	-1	3.65806	-5.05336	4.17599	L	H-H_	80	0.	0.
O-O_2	-1	-1.36081	8.20267	-4.36042	L				
O-O_2	-1	-3.87109	7.65028	-3.80934	L				

Si-Si3	-1	-2.88892	8.62181	-4.63487	L
O-O_2	-1	-6.00904	6.2315	-4.44246	L
Si-Si3	-1	-4.62037	6.23955	-3.62561	L
O-O_2	-1	1.26032	8.21442	-4.36295	L
Si-Si3	-1	2.78452	8.64722	-4.64034	L
O-O_2	-1	-0.03986	6.0363	-3.67733	L
Si-Si3	-1	-0.04701	7.6453	-3.6158	L
Si-Si3	-1	-7.31842	5.32498	-4.67375	L
O-O_2	-1	-3.67632	5.05215	-4.16781	L
O-O_2	-1	1.26468	8.2247	0.20308	L
Si-Si3	-1	2.7894	8.65874	0.4756	L
O-O_2	-1	-1.35294	8.22127	3.89647	L
O-O_2	-1	-3.86322	7.66887	4.44755	L
Si-Si3	-1	-2.88105	8.64041	3.62203	L
O-O_2	-1	-6.00117	6.25009	3.81443	L
Si-Si3	-1	-4.61249	6.25815	4.63153	L
O-O_2	-1	-6.00451	6.24219	0.30539	L
Si-Si3	-1	-4.6174	6.24656	-0.51439	L
O-O_2	-1	-1.35646	8.21296	0.2056	L
O-O_2	-1	-3.86778	7.65809	-0.33819	L
Si-Si3	-1	-2.88404	8.63333	0.48107	L
O-O_2	-1	1.2682	8.23301	3.89394	L
Si-Si3	-1	2.7924	8.66582	3.61656	L
O-O_2	-1	-0.03114	5.32401	2.05629	L
O-O_2	-1	-0.04767	8.1241	-2.07851	L
O-O_2	-1	3.12038	8.54614	2.04603	L
O-O_2	-1	-3.21097	8.51778	2.05213	L
O-O_2	-1	-4.94102	5.98748	-2.06903	L
O-O_2	-1	-0.0368	6.04353	-0.47024	L
Si-Si3	-1	-0.04407	7.65223	-0.53925	L
O-O_2	-1	-0.03198	6.0549	4.57956	L
Si-Si3	-1	-0.03913	7.6639	4.64134	L
Si-Si3	-1	-7.31054	5.34358	3.58339	L
Si-Si3	-1	-7.31344	5.33673	0.54301	L
O-O_2	-1	-3.66844	5.07075	4.08908	L
O-O_2	-1	-3.67231	5.06161	0.0316	L
O-O_2	-1	5.92585	6.28495	-4.45396	L
Si-Si3	-1	4.53918	6.28057	-3.63444	L
O-O_2	-1	3.77694	7.68453	-3.81672	L
Si-Si3	-1	7.24328	5.3902	-4.68779	L
O-O_2	-1	3.60461	5.08476	-4.17483	L
O-O_2	-1	3.78025	7.69235	-0.34557	L
O-O_2	-1	5.93038	6.29564	0.29388	L
Si-Si3	-1	4.54214	6.28758	-0.52322	L

O-O_2	-1	5.93373	6.30354	3.80293	L
Si-Si3	-1	4.54705	6.29917	4.6227	L
O-O_2	-1	3.78481	7.70312	4.44018	L
O-O_2	-1	4.86507	6.0314	-2.07849	L
Si-Si3	-1	7.25116	5.4088	3.56935	L
Si-Si3	-1	7.24826	5.40195	0.52897	L
O-O_2	-1	3.60861	5.09422	0.02458	L
O-O_2	-1	3.61248	5.10336	4.08206	L
H-H_	-1	-3.08969	9.83732	-4.24037	L
H-H_	-1	-3.08556	9.84706	0.08148	L
H-H_	-1	-3.08181	9.85592	4.01652	L
H-H_	-1	2.9748	9.86453	-4.2462	L
H-H_	-1	2.97892	9.87427	0.07562	L
H-H_	-1	2.98268	9.88313	4.0107	L
H-H_	-1	8.29594	6.11874	-4.50191	L
H-H_	-1	8.30058	6.12965	0.338	L
H-H_	-1	8.30384	6.13735	3.75504	L
H-H_	-1	10.88785	2.32933	-3.97279	L
H-H_	-1	10.89147	2.33788	-0.17893	L
H-H_	-1	10.89572	2.34793	4.2841	L
H-H_	-1	10.3603	1.63883	-5.89441	L
H-H_	-1	-8.3772	6.04406	-4.48583	L
H-H_	-1	-8.37261	6.05498	0.35407	L
H-H_	-1	-8.36935	6.06268	3.77111	L
H-H_	-1	-10.93447	2.2316	-3.95176	L
H-H_	-1	-10.93085	2.24014	-0.1579	L
H-H_	-1	-10.92659	2.2502	4.30514	L
H-H_	-1	-10.37854	-1.63996	5.90269	L
H-H_	-1	-10.90639	-2.33095	3.98097	L
H-H_	-1	-10.91001	-2.3395	0.18687	L
H-H_	-1	-10.91427	-2.34955	-4.27617	L
H-H_	-1	-8.32215	-6.13861	-3.7471	L
H-H_	-1	10.90805	-2.25181	-4.29721	L
H-H_	-1	10.91231	-2.24176	0.16583	L
H-H_	-1	10.91593	-2.23321	3.95994	L
H-H_	-1	10.38595	-1.54696	5.8826	L
H-H_	-1	8.35144	-6.06393	-3.76317	L
H-H_	-1	8.3547	-6.05624	-0.3459	L
H-H_	-1	8.35931	-6.04534	4.49372	L
H-H_	-1	3.07123	-9.83832	4.24835	L
H-H_	-1	3.1361	-8.52421	5.90531	L
H-H_	-1	-2.99325	-9.86543	4.25421	L
H-H_	-1	-3.06635	-8.55199	5.91129	L
H-H_	-1	-2.99737	-9.87516	-0.06753	L

H-H_	-1	-3.00113	-9.88409	-4.00275	L
H-H_	-1	3.0671	-9.84805	-0.07336	L
H-H_	-1	3.06336	-9.85698	-4.00861	L
H-H_	-1	4.85218	-6.05699	-5.87478	L
H-H_	-1	7.27568	-2.10182	-5.88856	L
H-H_	-1	0.02112	-8.05019	-5.86824	L
H-H_	-1	2.44506	-4.095	-5.8769	L
H-H_	-1	7.24403	4.9601	-5.9078	L
H-H_	-1	4.15768	1.61105	-5.88844	L
H-H_	-1	-2.43773	-4.11687	-5.87219	L
H-H_	-1	-4.82717	-6.10034	-5.86545	L
H-H_	-1	3.04821	8.551	-5.90311	L
H-H_	-1	-0.03826	5.20141	-5.90139	L
H-H_	-1	-7.28602	-2.16703	-5.87452	L
H-H_	-1	-4.20174	1.57361	-5.88045	L
H-H_	-1	-3.15418	8.52322	-5.89714	L
H-H_	-1	-7.31767	4.89489	-5.89376	L
H-H_	-1	-10.40413	1.54583	-5.87447	L
H-H_	-1	-7.29379	2.10078	5.89672	L
H-H_	-1	-4.8703	6.05549	5.88287	L
H-H_	-1	-0.03966	8.04861	5.87641	L
H-H_	-1	-2.46316	4.09389	5.885	L
H-H_	-1	-7.26214	-4.9613	5.91558	L
H-H_	-1	-4.17609	-1.61219	5.89671	L
H-H_	-1	2.41961	4.11576	5.88029	L
H-H_	-1	4.80907	6.09884	5.87354	L
H-H_	-1	0.01972	-5.20284	5.90918	L
H-H_	-1	4.18326	-1.57474	5.88858	L
H-H_	-1	7.26791	2.16599	5.88269	L
H-H_	-1	7.29956	-4.89609	5.90154	L
Al-Al3	0	2.62114	-4.02325	0.50948	H
H-H_	0	-0.03132	-2.39255	1.80367	H
C-C_3	0	-0.21993	-1.43442	1.31212	H
C-C_3	0	0.79558	-1.16433	0.19699	H
H-H_	0	-1.2469	-1.42063	0.93582	H
H-H_	0	-0.14023	-0.64719	2.0698	H
C-C_3	0	0.87898	-2.25292	-0.877	H
C-C_3	0	0.49863	0.15572	-0.53857	H
H-H_	0	-0.06213	-2.30792	-1.42704	H
H-H_	0	1.70016	-2.04942	-1.5648	H
H-H_	0	1.26187	0.37414	-1.29267	H
H-H_	0	-0.48183	0.12528	-1.03062	H
H-H_	0	0.4881	0.99501	0.16159	H
H-H_	0	1.78457	-1.07823	0.65158	H

S8. The coordinates for the adsorption of isobutene on HZSM-48

O-O_2	-1	-5.97438	-1.97428	-3.89564	L			
O-O_2	-1	-3.45925	-2.50664	-4.44428	L			
O-O_2	-1	-5.95227	-6.30455	-3.795	L			
Si-Si3	-1	-4.4501	-1.54024	-3.62311	L			
Si-Si3	-1	-4.56516	-6.30018	-4.61452	L			
O-O_2	-1	-1.34412	3.87136	-4.44159	L			
Si-Si3	-1	-2.73122	3.86699	-3.62207	L			
O-O_2	-1	-5.99217	1.90059	-4.34181	L			
O-O_2	-1	-3.48085	2.45546	-3.79801	L			
Si-Si3	-1	-4.46458	1.48022	-4.61728	L			
O-O_2	-1	-1.28674	-8.23402	-3.88601	L			
O-O_2	-1	-3.80292	-7.70413	-4.43225	L			
O-O_2	-1	-1.30868	-3.90334	-3.80484	L			
Si-Si3	-1	-2.8105	-8.66682	-3.60863	L			
Si-Si3	-1	-2.69735	-3.9114	-4.62168	L			
O-O_2	-1	-8.6133	1.88886	-4.33928	L			
O-O_2	-1	3.43326	2.48643	-3.80468	L			
Si-Si3	-1	-10.13803	1.45481	-4.61181	L			
O-O_2	-1	1.33439	-8.22228	-3.88854	L			
O-O_2	-1	1.31813	-3.89158	-3.80737	L			
Si-Si3	-1	2.86294	-8.64141	-3.6141	L			
Si-Si3	-1	2.70524	-3.88721	-4.62689	L			
O-O_2	-1	-8.59552	-1.98602	-3.89312	L			
O-O_2	-1	3.45486	-2.47567	-4.45095	L			
Si-Si3	-1	-10.12354	-1.56565	-3.61765	L			
O-O_2	-1	1.2827	3.88313	-4.44413	L			
Si-Si3	-1	2.67137	3.89119	-3.62728	L			
O-O_2	-1	-7.27586	-4.15485	-4.56896	L			
Si-Si3	-1	-7.26926	-5.41041	-3.56118	L			
Si-Si3	-1	-7.28313	-2.54615	-4.63772	L			
Si-Si3	-1	-0.03518	4.77682	-4.67946	L			
O-O_2	-1	-7.31183	4.07003	-3.66597	L			
Si-Si3	-1	-7.30455	2.46133	-3.5972	L			
O-O_2	-1	0.01344	-6.05652	-4.57163	L			
Si-Si3	-1	0.00876	-4.79642	-3.5695	L	H-H_	95	0. 0.
Si-Si3	-1	0.02059	-7.66551	-4.63316	L			
O-O_2	-1	-4.21401	-0.02892	-4.12043	L			
O-O_2	-1	-10.37367	-0.05651	-4.11449	L			
O-O_2	-1	-3.63074	-5.10456	-4.07413	L			
O-O_2	-1	1.31195	3.84986	0.29242	L			
Si-Si3	-1	2.71188	3.88772	-0.55504	L			
O-O_2	-1	-5.96651	-1.95569	4.3615	L			

O-O_2	-1	-3.45137	-2.48804	3.81286	L			
O-O_R	-1	-5.9444	-6.28595	4.46189	L			
Si-Si3	-1	-4.44222	-1.52164	4.63402	L			
Si-Si3	-1	-4.55729	-6.28158	3.64237	L			
O-O_2	-1	-1.33624	3.88996	3.8153	L			
Si-Si3	-1	-2.72335	3.88559	4.63507	L			
O-O_2	-1	-8.592	-1.97771	-0.20225	L			
O-O_3	0	3.46162	-2.29756	0.46943	H			
Si-Si3	-1	-10.12054	-1.55858	-0.47669	L			
O-O_2	-1	-5.98429	1.91919	3.91508	L			
O-O_2	-1	-3.47297	2.47406	4.45888	L			
Si-Si3	-1	-4.45671	1.49882	3.63961	L			
O-O_2	-1	1.33791	-8.21397	-0.19767	L			
O-O_2	0	1.2117	-3.78211	-0.47028	H			
Si-Si3	-1	2.86594	-8.63434	-0.47314	L			
O-O_2	-1	-8.60894	1.89914	0.22674	L			
O-O_2	-1	3.43377	2.44825	-0.37569	L	H-H_	163	0. 0.
Si-Si3	-1	-10.13314	1.46633	0.50413	L			
O-O_2	-1	-1.27887	-8.21542	4.37113	L			
O-O_2	-1	-3.79505	-7.68553	3.82489	L			
O-O_2	-1	-1.3008	-3.88474	4.45206	L			
Si-Si3	-1	-2.80263	-8.64822	4.64852	L			
Si-Si3	-1	-2.68947	-3.8928	3.6352	L			
O-O_2	-1	-8.60542	1.90745	3.91761	L			
O-O_2	-1	3.44114	2.50502	4.45221	L			
Si-Si3	-1	-10.13015	1.47341	3.64508	L			
O-O_2	-1	-1.28322	-8.2257	-0.19515	L			
O-O_2	-1	-3.79836	-7.69335	0.35349	L			
O-O_2	0	-1.40144	-3.86134	-0.36014	H			
Si-Si3	-1	-2.80751	-8.65975	-0.46767	L			
Si-Si3	-1	-2.74963	-3.91773	0.56113	H			
O-O_2	-1	-5.98781	1.91088	0.22422	L			
O-O_2	-1	-3.47754	2.46328	-0.32687	L			
Si-Si3	-1	-4.481	1.48075	0.50002	L			
O-O_2	-1	1.34227	-8.20368	4.3686	L			
O-O_2	-1	1.32601	-3.87298	4.44952	L	H-H_	80	0. 0.
Si-Si3	-1	2.87081	-8.62282	4.64305	L			
Si-Si3	0	2.71312	-3.8686	3.63001	H			
O-O_2	-1	-1.34468	3.84345	0.28372	L			
Si-Si3	-1	-2.75707	3.87568	-0.5464	L			
O-O_2	-1	-8.58764	-1.96743	4.36402	L			
O-O_2	-1	3.46274	-2.45707	3.80619	L	H-H_	80	0. 0.
Si-Si3	-1	-10.11566	-1.54705	4.63949	L			
O-O_2	-1	1.29057	3.90173	3.81277	L			

Si-Si3	-1	2.67924	3.90979	4.62986	L				
O-O_2	-1	-6.08416	-1.8723	-0.39229	L				
O-O_2	-1	-3.60323	-2.51667	0.48651	L	H-H_	73	0.	0.
O-O_R	-1	-5.94892	-6.29664	-0.2857	L				
Si-Si3	-1	-4.50172	-1.5615	-0.49395	L				
Si-Si3	-1	-4.56025	-6.28859	0.53114	L				
O-O_R	-1	-7.2702	-4.87436	-2.04235	L				
O-O_2	-1	-7.30961	4.80814	2.06439	L				
O-O_2	-1	-0.03782	-5.5026	-2.06961	H				
O-O_2	-1	-7.27885	-2.05567	2.07983	L				
O-O_2	-1	-7.30096	1.98945	-2.05778	L				
O-O_2	-1	0.02913	-8.12572	2.08653	L				
O-O_2	-1	-3.98872	-1.7521	-2.03159	L				
O-O_2	-1	-10.45046	-1.6812	-2.04651	L				
O-O_2	-1	-4.12978	1.61498	2.06855	L				
O-O_2	-1	3.19286	-8.51879	-2.04412	L				
O-O_2	-1	-10.46113	1.58662	2.07466	L				
O-O_2	-1	-3.13849	-8.54714	-2.03801	L				
O-O_2	-1	2.34844	4.14737	-2.07184	L				
O-O_2	-1	-4.88318	-6.03302	2.0865	L				
O-O_2	-1	-2.40761	4.12607	-2.06726	L				
O-O_2	0	2.22866	-4.14452	2.13262	H				
O-O_2	-1	-2.24564	-4.21334	2.07366	L	H-H_	73	0.	0.
Si-Si3	-1	-0.0258	4.76756	0.55282	L				
O-O_R	-1	-7.26798	-4.13625	3.68793	L				
Si-	-1	-7.26139	-5.39181	4.69572	L				
Si-Si3	-1	-7.27526	-2.52755	3.61917	L				
Si-Si3	-1	-0.02731	4.79542	3.57768	L				
O-O_R	-1	-7.27104	-4.14347	0.48109	L				
Si-	-1	-7.26637	-5.40356	-0.52104	L				
Si-Si3	-1	-7.27819	-2.53447	0.54262	L				
O-O_2	-1	-7.30395	4.08863	4.59093	L				
Si-Si3	-1	-7.29668	2.47993	4.65994	L				
O-O_2	-1	0.00666	-5.98223	0.54898	H				
Si-Si3	0	-0.04282	-4.79033	-0.60047	H				
Si-Si3	-1	0.02553	-7.65383	0.54718	L	H-H_	120	0.	0.
O-O_2	-1	-7.30877	4.07725	-0.45888	L				
Si-Si3	-1	-7.30162	2.46826	-0.52065	L				
O-O_2	-1	0.02132	-6.03792	3.68526	L				
Si-Si3	-1	0.01664	-4.77783	4.68739	L				
Si-Si3	-1	0.02846	-7.64691	3.62373	L				
O-O_2	-1	-4.20613	-0.01032	4.13646	L				
O-O_2	-1	-10.36974	-0.04721	0.01408	L				
O-O_2	-1	-10.3658	-0.03791	4.1424	L				

O-O_2	-1	-4.22151	-0.03194	-0.01742	L				
O-O_2	-1	-3.62286	-5.08597	4.18301	L				
O-O_2	-1	-3.64994	-5.08836	-0.13674	L	H-H_	73	0.	0.
O-O_2	-1	8.58732	-1.90907	-3.90968	L				
Si-Si3	-1	10.11161	-1.47502	-3.63715	L				
O-O_2	-1	8.56953	1.96581	-4.35585	L				
Si-Si3	-1	10.09712	1.54544	-4.63132	L				
O-O_2	-1	5.9484	1.95407	-4.35332	L				
Si-Si3	-1	4.42411	1.52003	-4.62585	L				
O-O_2	-1	3.8451	-7.66988	-4.43962	L				
O-O_2	-1	5.96619	-1.92081	-3.90715	L				
O-O_2	-1	5.98262	-6.2511	-3.8065	L				
Si-Si3	-1	4.43861	-1.50043	-3.63171	L	H-H_	180	0.	0.
Si-Si3	-1	4.59438	-6.25915	-4.62335	L				
O-O_2	-1	7.28584	-4.08963	-4.583	L				
Si-Si3	-1	7.29244	-5.34519	-3.57521	L				
Si-Si3	-1	7.27857	-2.48093	-4.65176	L				
O-O_2	-1	7.24988	4.13525	-3.68	L				
Si-Si3	-1	7.25715	2.52654	-3.61124	L				
O-O_2	-1	10.34769	0.0363	-4.13447	L				
O-O_2	-1	4.18803	0.00871	-4.12853	L				
O-O_2	-1	3.65019	-5.07195	-4.08115	L				
O-O_2	-1	8.5952	-1.89047	4.34746	L				
Si-Si3	-1	10.11948	-1.45642	4.61999	L				
O-O_2	-1	6.06404	-1.85361	-0.39998	H				
O-O_2	-1	5.98597	-6.24319	-0.29721	L				
Si-Si3	0	4.52093	-1.46397	-0.54527	H				
Si-Si3	-1	4.59928	-6.24755	0.52231	L	H-H_	198	0.	0.
O-O_2	-1	8.57741	1.98441	3.90105	L				
Si-Si3	-1	10.105	1.56403	3.62558	L				
O-O_2	-1	3.84967	-7.6591	0.34612	L				
O-O_2	-1	5.95276	1.96431	0.21271	L	H-H_	163	0.	0.
Si-Si3	-1	4.45654	1.54611	0.49373	H				
O-O_2	-1	5.95628	1.97267	3.90357	L				
Si-Si3	-1	4.43199	1.53863	3.63105	L				
O-O_2	-1	8.57389	1.9761	0.21018	L				
Si-Si3	-1	10.102	1.55696	0.48462	L				
O-O_2	-1	3.85298	-7.65128	3.81752	L				
O-O_2	-1	5.97406	-1.90221	4.34999	L				
O-O_2	-1	5.9905	-6.2325	4.45039	L				
Si-Si3	-1	4.44648	-1.48183	4.62546	L				
Si-Si3	-1	4.60226	-6.24056	3.63354	L				
O-O_2	-1	8.59084	-1.90075	-0.21881	L				
Si-Si3	-1	10.1146	-1.46795	-0.4962	L				

O-O_2	-1	7.2915	-4.80914	-2.05638	L				
O-O_2	-1	7.25209	4.87336	2.05036	L				
O-O_2	-1	7.28285	-1.99045	2.06579	L				
O-O_2	-1	7.26075	2.05467	-2.07181	L				
O-O_2	-1	10.44302	-1.58763	-2.06665	L				
O-O_2	-1	3.98214	-1.71211	-2.04598	H				
O-O_2	-1	10.43236	1.6802	2.05452	L				
O-O_2	-1	4.10057	1.65185	2.06063	L	H-H_	163	0.	0.
O-O_2	-1	4.92292	-5.9891	2.07705	L				
O-O_2	-1	7.29372	-4.07103	3.6739	L				
Si-Si3	-1	7.30031	-5.3266	4.68168	L				
Si-Si3	-1	7.28645	-2.46233	3.60513	L				
O-O_2	-1	7.29066	-4.07826	0.46705	L				
Si-Si3	-1	7.29534	-5.33835	-0.53508	L				
Si-Si3	-1	7.28351	-2.46926	0.52858	L	H-H_	155	0.	0.
O-O_2	-1	7.25775	4.15385	4.57689	L				
Si-Si3	-1	7.26502	2.54514	4.6459	L				
O-O_2	-1	7.25293	4.14247	-0.47291	L				
Si-Si3	-1	7.26007	2.5335	-0.53469	L				
O-O_2	-1	10.35557	0.0549	4.12242	L				
O-O_2	0	4.24006	0.0359	-0.04362	H				
O-O_2	-1	4.1959	0.02731	4.12836	L				
O-O_2	-1	10.35163	0.0456	-0.0059	L				
O-O_2	0	3.75852	-5.0662	-0.16924	H				
O-O_2	-1	3.65806	-5.05336	4.17599	L	H-H_	80	0.	0.
O-O_2	-1	-1.36081	8.20267	-4.36042	L				
O-O_2	-1	-3.87109	7.65028	-3.80934	L				
Si-Si3	-1	-2.88892	8.62181	-4.63487	L				
O-O_2	-1	-6.00904	6.2315	-4.44246	L				
Si-Si3	-1	-4.62037	6.23955	-3.62561	L				
O-O_2	-1	1.26032	8.21442	-4.36295	L				
Si-Si3	-1	2.78452	8.64722	-4.64034	L				
O-O_2	-1	-0.03986	6.0363	-3.67733	L				
Si-Si3	-1	-0.04701	7.6453	-3.6158	L				
Si-Si3	-1	-7.31842	5.32498	-4.67375	L				
O-O_2	-1	-3.67632	5.05215	-4.16781	L				
O-O_2	-1	1.26468	8.2247	0.20308	L				
Si-Si3	-1	2.7894	8.65874	0.4756	L				
O-O_2	-1	-1.35294	8.22127	3.89647	L				
O-O_2	-1	-3.86322	7.66887	4.44755	L				
Si-Si3	-1	-2.88105	8.64041	3.62203	L				
O-O_2	-1	-6.00117	6.25009	3.81443	L				
Si-Si3	-1	-4.61249	6.25815	4.63153	L				
O-O_2	-1	-6.00451	6.24219	0.30539	L				

Si-Si3	-1	-4.6174	6.24656	-0.51439	L
O-O_2	-1	-1.35646	8.21296	0.2056	L
O-O_2	-1	-3.86778	7.65809	-0.33819	L
Si-Si3	-1	-2.88404	8.63333	0.48107	L
O-O_2	-1	1.2682	8.23301	3.89394	L
Si-Si3	-1	2.7924	8.66582	3.61656	L
O-O_2	-1	-0.03114	5.32401	2.05629	L
O-O_2	-1	-0.04767	8.1241	-2.07851	L
O-O_2	-1	3.12038	8.54614	2.04603	L
O-O_2	-1	-3.21097	8.51778	2.05213	L
O-O_2	-1	-4.94102	5.98748	-2.06903	L
O-O_2	-1	-0.0368	6.04353	-0.47024	L
Si-Si3	-1	-0.04407	7.65223	-0.53925	L
O-O_2	-1	-0.03198	6.0549	4.57956	L
Si-Si3	-1	-0.03913	7.6639	4.64134	L
Si-Si3	-1	-7.31054	5.34358	3.58339	L
Si-Si3	-1	-7.31344	5.33673	0.54301	L
O-O_2	-1	-3.66844	5.07075	4.08908	L
O-O_2	-1	-3.67231	5.06161	0.0316	L
O-O_2	-1	5.92585	6.28495	-4.45396	L
Si-Si3	-1	4.53918	6.28057	-3.63444	L
O-O_2	-1	3.77694	7.68453	-3.81672	L
Si-Si3	-1	7.24328	5.3902	-4.68779	L
O-O_2	-1	3.60461	5.08476	-4.17483	L
O-O_2	-1	3.78025	7.69235	-0.34557	L
O-O_2	-1	5.93038	6.29564	0.29388	L
Si-Si3	-1	4.54214	6.28758	-0.52322	L
O-O_2	-1	5.93373	6.30354	3.80293	L
Si-Si3	-1	4.54705	6.29917	4.6227	L
O-O_2	-1	3.78481	7.70312	4.44018	L
O-O_2	-1	4.86507	6.0314	-2.07849	L
Si-Si3	-1	7.25116	5.4088	3.56935	L
Si-Si3	-1	7.24826	5.40195	0.52897	L
O-O_2	-1	3.60861	5.09422	0.02458	L
O-O_2	-1	3.61248	5.10336	4.08206	L
H-H_	-1	-3.08969	9.83732	-4.24037	L
H-H_	-1	-3.08556	9.84706	0.08148	L
H-H_	-1	-3.08181	9.85592	4.01652	L
H-H_	-1	2.9748	9.86453	-4.2462	L
H-H_	-1	2.97892	9.87427	0.07562	L
H-H_	-1	2.98268	9.88313	4.0107	L
H-H_	-1	8.29594	6.11874	-4.50191	L
H-H_	-1	8.30058	6.12965	0.338	L
H-H_	-1	8.30384	6.13735	3.75504	L

H-H_	-1	10.88785	2.32933	-3.97279	L
H-H_	-1	10.89147	2.33788	-0.17893	L
H-H_	-1	10.89572	2.34793	4.2841	L
H-H_	-1	10.3603	1.63883	-5.89441	L
H-H_	-1	-8.3772	6.04406	-4.48583	L
H-H_	-1	-8.37261	6.05498	0.35407	L
H-H_	-1	-8.36935	6.06268	3.77111	L
H-H_	-1	-10.93447	2.2316	-3.95176	L
H-H_	-1	-10.93085	2.24014	-0.1579	L
H-H_	-1	-10.92659	2.2502	4.30514	L
H-H_	-1	-10.37854	-1.63996	5.90269	L
H-H_	-1	-10.90639	-2.33095	3.98097	L
H-H_	-1	-10.91001	-2.3395	0.18687	L
H-H_	-1	-10.91427	-2.34955	-4.27617	L
H-H_	-1	-8.32215	-6.13861	-3.7471	L
H-H_	-1	10.90805	-2.25181	-4.29721	L
H-H_	-1	10.91231	-2.24176	0.16583	L
H-H_	-1	10.91593	-2.23321	3.95994	L
H-H_	-1	10.38595	-1.54696	5.8826	L
H-H_	-1	8.35144	-6.06393	-3.76317	L
H-H_	-1	8.3547	-6.05624	-0.3459	L
H-H_	-1	8.35931	-6.04534	4.49372	L
H-H_	-1	3.07123	-9.83832	4.24835	L
H-H_	-1	3.1361	-8.52421	5.90531	L
H-H_	-1	-2.99325	-9.86543	4.25421	L
H-H_	-1	-3.06635	-8.55199	5.91129	L
H-H_	-1	-2.99737	-9.87516	-0.06753	L
H-H_	-1	-3.00113	-9.88409	-4.00275	L
H-H_	-1	3.0671	-9.84805	-0.07336	L
H-H_	-1	3.06336	-9.85698	-4.00861	L
H-H_	-1	4.85218	-6.05699	-5.87478	L
H-H_	-1	7.27568	-2.10182	-5.88856	L
H-H_	-1	0.02112	-8.05019	-5.86824	L
H-H_	-1	2.44506	-4.095	-5.8769	L
H-H_	-1	7.24403	4.9601	-5.9078	L
H-H_	-1	4.15768	1.61105	-5.88844	L
H-H_	-1	-2.43773	-4.11687	-5.87219	L
H-H_	-1	-4.82717	-6.10034	-5.86545	L
H-H_	-1	3.04821	8.551	-5.90311	L
H-H_	-1	-0.03826	5.20141	-5.90139	L
H-H_	-1	-7.28602	-2.16703	-5.87452	L
H-H_	-1	-4.20174	1.57361	-5.88045	L
H-H_	-1	-3.15418	8.52322	-5.89714	L
H-H_	-1	-7.31767	4.89489	-5.89376	L

H-H_	-1	-10.40413	1.54583	-5.87447	L
H-H_	-1	-7.29379	2.10078	5.89672	L
H-H_	-1	-4.8703	6.05549	5.88287	L
H-H_	-1	-0.03966	8.04861	5.87641	L
H-H_	-1	-2.46316	4.09389	5.885	L
H-H_	-1	-7.26214	-4.9613	5.91558	L
H-H_	-1	-4.17609	-1.61219	5.89671	L
H-H_	-1	2.41961	4.11576	5.88029	L
H-H_	-1	4.80907	6.09884	5.87354	L
H-H_	-1	0.01972	-5.20284	5.90918	L
H-H_	-1	4.18326	-1.57474	5.88858	L
H-H_	-1	7.26791	2.16599	5.88269	L
H-H_	-1	7.29956	-4.89609	5.90154	L
Al-Al3	0	2.62114	-4.02325	0.50948	H
H-H_	0	-0.30701	-0.05053	-3.06606	H
C-C_3	0	-0.75511	0.26198	-2.11782	H
C-C_2	0	0.11321	-0.1081	-0.94337	H
H-H_	0	-0.90174	1.34892	-2.14579	H
H-H_	0	-1.74782	-0.18935	-2.03175	H
C-C_2	0	1.3063	-0.70155	-1.10258	H
C-C_3	0	-0.40355	0.27353	0.41905	H
H-H_	0	1.71521	-0.92774	-2.08251	H
H-H_	0	1.9697	-0.85426	-0.25678	H
H-H_	0	-0.53674	1.35915	0.4844	H
H-H_	0	-1.38291	-0.1796	0.60716	H
H-H_	0	0.28624	-0.03713	1.20838	H
H-H_	0	1.18906	-2.73744	-0.51113	H