

Supplementary material

QSAR modeling of corneal permeability of drugs – the application of Monte Carlo optimization method

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Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – Expr, the values of Ac calculated with the application of CORAL software – Calc, the difference between Expr and Calc – Diff for the built QSPR model.

SMILES notation	Expr	Split 1				Split 2				Split 3				
		DCW	Calc	Diff	Set	DCW	Calc	Diff	Set	DCW	Calc	Diff	Set	
1	<chem>CC(=O)Nc1nnc(s1)S(=O)(=O)N</chem>	-6.04	0.19311	-6.0385	-0.0015	Ts	19.85779	-6.1291	0.0891	Tr	-1.45422	-6.1922	0.1522	Tr
2	<chem>C=CCc1cccc1OCC(CNC(C)C)O</chem>	-4.54	66.86635	-4.3186	-0.2214	Tr	76.99438	-4.4167	-0.1233	Tr	44.06187	-4.58	0.04	Ts
3	<chem>OC(COc1ccc(cc1)CC(=O)N)CNC(C)C</chem>	-6.17	20.51512	-5.5143	-0.6557	Tr	29.64402	-5.8358	-0.3342	Tr	17.28472	-5.5285	-0.6415	Ts
4	<chem>O=S(=O)(c1cccc1)Nc1nnc(s1)S(=O)(=O)N</chem>	-6.85	-9.49742	-6.2885	-0.5615	Ts	-5.49106	-6.8888	0.0388	Tr	-11.4317	-6.5456	-0.3044	Ts
5	<chem>COc1cc(CCNCC(CO2cccc(c2)C)O)ccc1OC</chem>	-4.27	72.22556	-4.1803	-0.0897	Tr	82.6559	-4.247	-0.023	Tr	60.77589	-3.988	-0.282	Tr
6	<chem>CC(=O)N(c1nnc(s1)S(=O)(=O)N)Br</chem>	-6.42	-0.21864	-6.0491	-0.3709	Ts	10.39161	-6.4128	-0.0072	Tr	-2.62511	-6.2337	-0.1863	Tr
7	<chem>CCc1cccc2c1oc(c2)C(CNC(C)C)C)O</chem>	-4.24	71.85127	-4.19	-0.05	Tr	86.70648	-4.1256	-0.1144	Tr	50.53906	-4.3506	0.1106	Tr
8	<chem>Clc1cccc1c1nnc(s1)S(=O)(=O)N</chem>	-4.74	66.80806	-4.3201	-0.4199	Tr	74.76417	-4.4835	-0.2565	Tr	34.06971	-4.9339	0.1939	Ts
9	<chem>Clc1cccc(c1NC1=NCCN1)Cl</chem>	-4.51	56.72623	-4.5802	0.0702	Tr	69.76663	-4.6333	0.1233	Ts	39.82207	-4.7302	0.2202	Tr
11	<chem>C1CCN(P1(=O)NCCCO1)CCCl</chem>	-4.96	29.33495	-5.2868	0.3268	Ts	55.52814	-5.06	0.1	Ts	30.37475	-5.0648	0.1048	Tr
12	<chem>CCOc1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>	-4.25	47.9722	-4.806	0.556	Tr	71.85739	-4.5706	0.3206	Ts	36.23585	-4.8572	0.6072	Tr
13	<chem>NS(=O)(=O)c1nc2c(s1)cccc2</chem>	-4.44	53.17064	-4.6719	0.2319	Ts	71.26807	-4.5883	0.1483	Tr	40.2906	-4.7136	0.2736	Tr
14	<chem>Oc1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>	-5.25	39.63465	-5.0211	-0.2289	Ts	47.22552	-5.3089	0.0589	Tr	27.82316	-5.1552	-0.0948	Tr
15	<chem>Clc1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>	-4.37	67.58364	-4.3001	-0.0699	Tr	76.47008	-4.4324	0.0624	Tr	51.9525	-4.3005	-0.0695	Tr
16	<chem>Clc1cc(Cl)c2c(c1)sc(n2)S(=O)(=O)N</chem>	-4.41	54.43009	-4.6394	0.2294	Tr	76.29683	-4.4376	0.0276	Tr	47.60108	-4.4547	0.0447	Tr
17	<chem>Nc1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>	-5.17	37.11758	-5.086	-0.084	Tr	45.8739	-5.3494	0.1794	Ts	24.71838	-5.2652	0.0952	Tr
18	<chem>[O-][N+](=O)c1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>	-5.18	32.37731	-5.2083	0.0283	Tr	55.56161	-5.059	-0.121	Tr	21.3703	-5.3837	0.2037	Tr
19	<chem>OCCOc1ccc2c(c1)sc(n2)S(=O)(=O)N</chem>	-5.82	27.74422	-5.3278	-0.4922	Tr	57.80403	-4.9918	-0.8282	Tr	28.12437	-5.1445	-0.6755	Tr
20	<chem>c1ccc(cc1)COc1ccc2c(c1)scn2</chem>	-4.33	56.07864	-4.5969	0.2669	Ts	89.81447	-4.0324	-0.2976	Tr	45.14302	-4.5417	0.2117	Ts
21	<chem>CC(=O)Nc1ccc2c(c1)scn2</chem>	-5.33	34.4589	-5.1546	-0.1754	Tr	53.16071	-5.131	-0.199	Ts	30.82577	-5.0488	-0.2812	Tr
22	<chem>OC(COc1ccc2c1CC2=O)CNC(C)C)C</chem>	-4.7	46.19212	-4.8519	0.1519	Tr	63.49704	-4.8212	0.1212	Tr	41.9689	-4.6541	-0.0459	Tr
23	<chem>CC(CCc1cccc1)NCC(c1ccc(c1)C(=O)N)O)O</chem>	-4.85	36.66973	-5.0975	0.2475	Tr	55.69393	-5.0551	0.2051	Tr	28.28305	-5.1389	0.2889	Tr

24	CC(=O)N=c1sc(nn1C)S(=O)(=O)N	-5.59	17.92792	-5.581	-0.009	Ts	30.89194	-5.7984	0.2084	Tr	11.75755	-5.7242	0.1342	Ts
25	N=c1sc(nn1C)S(=O)(=O)N	-6.11	-1.2997	-6.077	-0.033	Tr	20.00129	-6.1248	0.0148	Tr	10.30364	-5.7757	-0.3343	Ts
26	COCCc1ccc(cc1)OCC(CNC(C)C)O	-4.6	50.09122	-4.7513	0.1513	Ts	68.03703	-4.6851	0.0851	Tr	41.59758	-4.6673	0.0673	Tr
27	OC(COc1ccc2c1CC(O)C(C2)O)CNC(C)C	-6	17.94811	-5.5805	-0.4195	Ts	31.74672	-5.7728	-0.2272	Ts	7.67518	-5.8688	-0.1312	Tr
28	C=CCOc1ccc1OCC(CNC(C)C)O	-4.54	58.36796	-4.5378	-0.0022	Ts	72.48199	-4.5519	0.0119	Tr	36.81994	-4.8365	0.2965	Ts
29	OC(COc1ccc1C1CCCC1)CNC(C)C	-4.35	66.31888	-4.3327	-0.0173	Tr	80.04353	-4.3253	-0.0247	Ts	59.94217	-4.0175	-0.3325	Tr
30	CNCC(c1ccc(c1)O)O	-6.03	0.32585	-6.0351	0.0051	Tr	27.98942	-5.8854	-0.1446	Tr	1.97838	-6.0706	0.0406	Tr
31	OC(COc1ccc2c1cc[nH]2)CNC(C)C	-5	43.31456	-4.9261	-0.0739	Ts	52.77625	-5.1425	0.1425	Tr	38.42964	-4.7795	-0.2205	Ts
32	OC(COc1ccc2c1ccc2)CNC(C)C	-4.32	67.34634	-4.3062	-0.0138	Tr	74.46341	-4.4925	0.1725	Tr	46.59454	-4.4903	0.1703	Tr
33	CCC1C2CC3N(C1O)C1C2C(O)C2(C3N(C)c3c2ccc3)C1	-5.04	36.24255	-5.1086	0.0686	Tr	53.05794	-5.1341	0.0941	Tr	30.37402	-5.0648	0.0248	Tr
34	C1NCCc2c1c1nnc1cc2	-4.1	77.61521	-4.0413	-0.0587	Tr	88.01274	-4.0864	-0.0136	Tr	56.65357	-4.134	0.034	Tr
35	CN1CCc2c(CC1)ccc2C1	-4.15	79.76128	-3.9859	-0.1641	Tr	82.56097	-4.2498	0.0998	Tr	56.22932	-4.149	-0.001	Ts
36	COc1ccc(c2c1CNCC2)OC	-4.31	64.8508	-4.3706	0.0606	Tr	73.52686	-4.5206	0.2106	Tr	46.76162	-4.4844	0.1744	Tr
37	CC(NCC(c1ccc(cc1)NS(=O)(=O)C)O)C	-5.8	10.98677	-5.7601	-0.0399	Tr	32.74071	-5.743	-0.057	Ts	24.8006	-5.2622	-0.5378	Ts
38	CNS(=O)(=O)c1ccc(cc1)Cl	-4.19	60.52976	-4.482	0.292	Tr	80.04832	-4.3251	0.1351	Tr	50.25512	-4.3607	0.1707	Tr
39	Cc1ccc(cc1)S(=O)(=O)N	-4.26	64.74029	-4.3734	0.1134	Tr	66.42765	-4.7334	0.4734	Tr	52.54871	-4.2794	0.0194	Tr
40	NS(=O)(=O)c1nn2c(s1)nsc2=Ne1ccc1	-5.1	34.04838	-5.1652	0.0652	Tr	65.39563	-4.7643	-0.3357	Tr	33.96997	-4.9375	-0.1625	Tr
41	Clc1ccc(c1)N=c1snc2n1nc(s2)S(=O)(=O)N	-4.89	42.69284	-4.9422	0.0522	Tr	62.45134	-4.8525	-0.0375	Ts	42.22895	-4.6449	-0.2451	Tr
42	Clc1ccc(cc1)N=c1snc2n1nc(s2)S(=O)(=O)N	-5.08	42.78846	-4.9397	-0.1403	Tr	59.3523	-4.9454	-0.1346	Tr	29.08384	-5.1105	0.0305	Tr
43	COc1ccc(c1)N=c1snc2n1nc(s2)S(=O)(=O)N	-5.35	28.60326	-5.3056	-0.0444	Tr	44.26371	-5.3976	0.0476	Tr	18.21191	-5.4956	0.1456	Tr
44	COc1ccc(cc1)N=c1snc2n1nc(s2)S(=O)(=O)N	-5.28	23.18862	-5.4453	0.1653	Ts	40.39162	-5.5137	0.2337	Ts	18.0572	-5.5011	0.2211	Ts
45	Oc1ccc(cc1)N=c1snc2n1nc(s2)S(=O)(=O)N	-6.46	15.97544	-5.6314	-0.8286	Ts	24.53571	-5.9889	-0.4711	Tr	5.65051	-5.9405	-0.5195	Tr
46	Fc1ccc(c1)N=c1snc2n1nc(s2)S(=O)(=O)N	-5.19	21.93295	-5.4777	0.2877	Tr	47.02338	-5.3149	0.1249	Tr	27.05966	-5.1822	-0.0078	Tr
47	Fc1ccc(cc1)N=c1snc2n1nc(s2)S(=O)(=O)N	-5.39	23.03353	-5.4493	0.0593	Tr	41.64237	-5.4762	0.0862	Tr	15.27545	-5.5996	0.2096	Tr
48	CN(c1ccc(cc1)N=c1snc2n1nc(s2)S(=O)(=O)N)C	-5.24	28.74932	-5.3019	0.0619	Tr	38.22823	-5.5785	0.3385	Tr	16.39986	-5.5598	0.3198	Tr
49	OC(COc1nsc1N1CCOCC1)CNC(C)C	-4.92	35.94295	-5.1163	0.1963	Tr	56.63792	-5.0268	0.1068	Ts	33.08174	-4.9689	0.0489	Tr
50	CC(=O)N=c1sc(nn1C(Cl)(Cl)Cl)S(=O)(=O)N	-4.96	48.61134	-4.7895	-0.1705	Tr	58.61531	-4.9675	0.0075	Tr	35.59987	-4.8797	-0.0803	Tr
51	CC(=O)N=c1sc(nn1C(F)(F)F)S(=O)(=O)N	-5.41	28.63149	-5.3049	-0.1051	Ts	40.80137	-5.5014	0.0914	Ts	22.9651	-5.3273	-0.0827	Ts
52	COC(=O)C1C(O)CCC2C1CC1N(C2)CCc2c1[nH]c1c2ccc1	-4.74	56.87182	-4.5764	-0.1636	Tr	64.10721	-4.8029	0.0629	Ts	42.58807	-4.6322	-0.1078	Tr
53	CCn1nc(C(=O)O)c(=O)c2c1cc1OCoc1c2	-5.82	18.68552	-5.5615	-0.2585	Tr	29.66104	-5.8353	0.0153	Tr	9.52373	-5.8033	-0.0167	Tr
54	CCn1cc(C(=O)O)c(=O)c2c1nc(C)cc2	-4.77	43.82398	-4.913	0.143	Tr	60.97123	-4.8969	0.1269	Ts	28.23791	-5.1405	0.3705	Ts

55	<chem>CCn1cc(C(=O)O)c(=O)e2e1nc(N1CCNCC1)c(e2)F</chem>	-5.77	13.23596	-5.7021	-0.0679	Tr	40.56275	-5.5085	-0.2615	Ts	15.36713	-5.5964	-0.1736	Tr
56	<chem>CCn1cc(C(=O)O)c(=O)e2e1cc(N1CCNCC1)c(e2)F</chem>	-5.85	12.48946	-5.7213	-0.1287	Tr	37.87206	-5.5892	-0.2608	Ts	7.11843	-5.8885	0.0385	Tr
58	<chem>Fc1cc2c(cc1N1CCNCC1)n(cc(e2=O)C(=O)O)C1CC1</chem>	-5.89	-3.42876	-6.1319	0.2419	Tr	38.04329	-5.5841	-0.3059	Tr	3.91376	-6.0021	0.1121	Tr
59	<chem>COc1c(N2CC3C(C2)CCCN3)c(F)cc2e1n(cc(e2=O)C(=O)O)C1CC1</chem>	-5.04	40.58302	-4.9966	-0.0434	Tr	47.08579	-5.313	0.273	Tr	31.6996	-5.0179	-0.0221	Tr
60	<chem>CN1CCN(CC1)c1c(F)cc2e3e1OCC(n3cc(e2=O)C(=O)O)C</chem>	-5.54	12.6222	-5.7179	0.1779	Tr	38.53765	-5.5692	0.0292	Tr	13.97221	-5.6458	0.1058	Tr
61	<chem>COc1c(N2CCNC(C2)C)c(F)cc2e1n(cc(e2=O)C(=O)O)C1CC1</chem>	-5.6	18.58314	-5.5641	-0.0359	Ts	35.78196	-5.6518	0.0518	Tr	15.30416	-5.5986	-0.0014	Ts
62	<chem>CCn1cc(C(=O)O)c(=O)e2e1c(F)c(N1CCNC(C1)C)c(e2)F</chem>	-5.46	14.49586	-5.6696	0.2096	Tr	36.34257	-5.635	0.175	Tr	22.34584	-5.3492	-0.1108	Tr
63	<chem>O=C1CC2(CCCC2)CC(=O)N1CCCCN1CCN(CC1)c1ncccn1</chem>	-4.18	70.6394	-4.2213	0.0413	Tr	89.78319	-4.0334	-0.1466	Tr	56.3868	-4.1435	-0.0365	Tr
64	<chem>Nc1cc(Cl)c(c(c1)Cl)NC1=NCCN1</chem>	-5.42	30.12014	-5.2665	-0.1535	Tr	46.12478	-5.3418	-0.0782	Tr	26.58388	-5.1991	-0.2209	Tr
65	<chem>Oc1ccc2c(c1)Oe1c(C32OC(=O)c2c3ccccc2)ccc(c1)O</chem>	-4.8	52.2452	-4.6958	-0.1042	Ts	60.39418	-4.9142	0.1142	Tr	38.86688	-4.764	-0.036	Ts
66	<chem>CCC1C(=O)OCC1Cc1cncn1C</chem>	-5.01	45.45159	-4.871	-0.139	Tr	60.87341	-4.8998	-0.1102	Tr	33.22806	-4.9637	-0.0463	Tr
67	<chem>NC(=O)Cc1ccc(c1N)C(=O)c1ccccc1</chem>	-4.13	66.39199	-4.3308	0.2008	Tr	78.42361	-4.3738	0.2438	Tr	56.85974	-4.1267	-0.0033	Tr
68	<chem>OC(COc1ccc(cc1)CCOCC1CC1)CNC(C)C</chem>	-4.22	56.45602	-4.5871	0.3671	Tr	79.57738	-4.3393	0.1193	Ts	41.47635	-4.6716	0.4516	Ts
69	<chem>OCC(=O)C1(O)C(C)CC2C1(C)CC(O)C1(C2CCC2=CC(=O)C=CC12C)F</chem>	-5.04	40.15433	-5.0077	-0.0323	Tr	61.27697	-4.8877	-0.1523	Tr	29.99189	-5.0784	0.0384	Tr

Table S2. The list of SAKs together with their correlation weights for the three runs of the Monte Carlo optimization.

SAk	CW(SAk)			SAk	CW(SAk)			SAk	CW(SAk)			SAk	CW(SAk)		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
00001000000	1.274	0.1032	1.96681	P2E0N...3-.	-1.4812	-1.31587	-1.7776	S3E0C...14-.	0.44564	1.64953	-0.91923	VS2-Br..6...	0.19789	-0.36443	1.33121
00010000000	-0.30036	2.11413	0.19169	P2E0O...0-.	0.34078	2.29019	-0.6932	S3E0C...15-.	-1.99848	-0.74092	-0.93826	VS2-Cl..4...	1.26469	2.33226	2.00812
00010000100	1.37421	-0.26425	2.45503	P2E0O...1-.	0.01155	-0.57607	-0.69213	S3E0C...16-.	0.67759	-0.11618	-0.45334	VS2-Cl..5...	0.14002	2.33351	1.39607
00011000000	0.34394	2.23622	0.66835	P2E0O...2-.	0.48072	0.15408	0.08716	S3E0C...17-.	-1.12647	0.6056	-1.63625	VS2-N...10..	-0.66603	-0.65881	-0.92023
10001000000	5.7547	3.11197	5.83166	P2E0O...3-.	-0.95707	2.15298	-1.01294	S3E0C...2-.	-0.98443	1.38505	-3.06419	VS2-N...11..	1.15639	-0.62183	-0.5221
10001001000	1.1416	-0.83269	2.35988	P2E0S...1-.	0.00826	0.38622	-0.73942	S3E0C...18-.	0.09075	-0.81336	0.02913	VS2-N...12..	-0.53551	-0.58821	-0.75241
10010000100	2.12635	1.12654	0.20811	P2E0S...2-.	0.30889	1.10364	0.18874	S3E0C...19-.	0.88994	0.13725	-0.14267	VS2-N...13..	0.15954	0.07694	0.3318
10011000000	-1.663	2.46527	-4.60318	P2E0o...2-.	0.39237	2.00671	0.56053	S3E0C...21-.	0.28896	-0.04734	-0.08937	VS2-N...14..	0.11163	-0.80028	2.23133
10011001000	-0.73869	-0.53421	0.05964	P2E0s...1-.	-1.86276	-0.31292	-3.56537	S3E0C...22-.	-0.81424	0.44335	0.32228	VS2-N...3...	-0.34118	-0.8923	-0.93073
10011100000	0.46632	1.09524	-0.068	P2E0s...2-.	0.37368	-0.37066	0.25741	S3E0C...23-.	0.6896	-0.30319	2.18737	VS2-N...4...	-0.19381	0.41273	-0.10519
10011100010	0.02181	-0.60736	-0.70387	P3E0C...0-.	0.33024	0.10022	0.31375	S3E0C...24-.	2.03587	0.3233	-0.04864	VS2-N...5...	0.33791	2.12598	0.43886
10011100100	2.20173	2.02994	2.4146	P3E0C...1-.	2.09031	0.17218	0.04277	S3E0C...25-.	1.23905	0.11149	-0.10697	VS2-N...6...	2.31613	0.291	-0.74318
10011101000	0.45966	-0.6015	-0.85083	P3E0C...2-.	0.23298	0.04083	-0.456	S3E0C...3-.	0.48521	2.08839	0.47973	VS2-N...7...	-0.59219	-0.68973	1.27198
(...C.....)	0.31083	0.18215	0.45099	P3E0C...3-.	-0.47227	-1.59349	-1.78076	S3E0C...4-.	-0.22418	-0.54045	-0.27889	VS2-N...8...	0.3806	0.06074	0.66103
(.....)	-0.71345	-0.59678	-0.51236	P3E0C...4-.	-0.55611	-0.54204	-0.6173	S3E0C...5-.	0.24318	0.43773	0.27768	VS2-N...9...	-0.12383	0.24948	-0.52627
(...C...(...	-0.95832	2.21307	0.04679	P3E0C...5-.	0.27803	0.10577	-0.68751	S3E0C...6-.	-0.12379	0.25755	0.14952	VS2-O...10..	0.02308	0.22019	-0.8205
(...F...(...	2.17058	-0.69057	0.04087	P3E0C...6-.	-0.5187	0.1436	-0.84493	S3E0C...7-.	0.68226	0.33699	0.44544	VS2-O...13..	0.50564	0.84112	-0.78969
(...Cl...(...	2.1063	0.2897	-0.53918	P3E0C...7-.	0.51004	-0.84694	0.50892	S3E0C...8-.	0.08821	0.31078	0.39776	VS2-O...2...	-1.10246	-0.77705	-1.41404
(...N...(...	-0.08282	0.01928	-0.5112	P3E0C...8-.	0.24064	0.4784	0.18537	S3E0C...9-.	0.40924	0.2429	2.13831	VS2-O...3...	-0.75548	-0.70574	2.31311
(...O...(...	0.18161	-0.25598	-0.77102	P3E0F...1-.	0.36464	0.24578	0.33702	S3E0F...11-.	0.11953	-0.6893	-0.68661	VS2-O...4...	0.20391	-0.56788	0.35179
(...S...(...	2.0346	-0.87078	-0.13308	P3E0F...2-.	0.16316	0.68498	0.37234	S3E0F...13-.	2.68047	0.92008	0.1878	VS2-O...5...	0.04246	0.3331	-0.46955
(...c...(...	0.23509	0.16416	0.38741	P3E0F...3-.	0.03525	1.01755	-0.83077	S3E0F...3-.	-0.0325	0.49407	0.73324	VS2-O...6...	0.17392	0.17121	0.19848
(...n...(...	-0.99215	-0.83327	-1.34535	P3E0F...6-.	2.11295	-0.52727	-0.04836	S3E0F...4-.	-0.32418	1.23867	-0.52245	VS2-O...7...	0.30336	-0.8242	-1.05821
++++F---B2==	1.19009	-0.30137	0.36338	P3E0Br..3-.	-0.42701	-0.30044	-0.97579	S3E0F...7-.	-0.27387	-0.9996	0.24129	VS2-O...8...	1.20396	0.73216	2.43346
++++F---N===	0.10882	-0.80166	1.98738	P3E0Cl..1-.	0.10379	0.05239	2.44224	S3E0F...8-.	0.4998	-0.58746	0.1181	VS2-O...9...	0.43808	-0.96875	-0.53864
++++F---O===	0.10822	-0.02877	-0.75125	P3E0Cl..2-.	-1.21006	2.46042	-1.91578	S3E0Br..5-.	0.30019	-0.96466	0.56442	VS2-S...4...	0.32909	0.18224	-0.86802
++++F---S===	-0.81107	0.61788	1.89555	P3E0N...0-.	-0.96539	-0.44348	-0.22167	S3E0Cl..3-.	0.08447	0.27916	2.01828	VS2-S...5...	2.32444	2.08515	2.41221
++++CL--N===	2.71268	-0.04167	1.58909	P3E0N...1-.	0.22465	0.31511	0.43627	S3E0Cl..4-.	-1.17263	0.8193	-0.23001	VS2-S...7...	-0.77066	-0.90769	0.03829
++++CL--O===	2.09718	0.02125	1.09544	P3E0N...2-.	-0.97331	0.20544	0.34293	S3E0Cl..5-.	-0.40119	2.1295	1.24006	VS2-o...11..	2.5092	2.35953	4.05084
++++CL--S===	-0.49883	2.1228	2.25014	P3E0N...3-.	0.18547	-0.95994	0.14027	S3E0Cl..6-.	0.40214	2.07524	0.27635	VS2-s...10..	-0.5079	0.25327	0.05789
++++Br--B2==	0.45093	-0.90783	0.2589	P3E0N...4-.	-0.94114	-0.55611	0.33567	S3E0Cl..7-.	0.33827	0.01215	-0.28162	VS2-s...11..	-0.11082	0.13836	0.60672
++++Br--N===	-1.66469	-0.0559	0.03301	P3E0N...5-.	0.4188	0.47444	2.00934	S3E0N...1-.	0.44568	-0.5967	2.14601	VS2-s...7...	-0.02919	0.59638	-1.04991

++++Br--O===	-0.81243	1.4587	0.42437	P3E0N...6-.	-0.91079	-0.77738	-0.57825	S3E0N...10-.	0.34342	1.37335	2.49671	VS2-s...8...	-0.4078	-0.00906	-0.09146
++++Br--S===	0.46672	-0.53659	0.33788	P3E0N...7-.	1.2186	2.38216	-0.68271	S3E0N...11-.	-0.06659	0.23786	-0.80895	VS3-C...10..	0.10775	0.37438	-0.90557
++++Cl--B2==	2.4197	-0.10638	2.97367	P3E0O...0-.	0.32061	-0.23119	0.04165	S3E0N...12-.	0.42543	-0.10909	-0.51109	VS3-C...11..	2.14745	1.23269	0.12604
++++N--B2==	5.61119	0.10733	-0.17045	P3E0O...1-.	0.24612	-0.97559	-0.96866	S3E0N...13-.	1.19381	-0.65987	0.36133	VS3-C...12..	0.37116	0.13876	1.1707
++++N--O===	-0.79562	-0.77154	0.12613	P3E0O...2-.	-4.03841	-1.06281	-3.57496	S3E0N...15-.	0.2162	-0.10446	0.43071	VS3-C...13..	0.13211	0.21377	0.56851
++++N--S===	-0.33215	0.18703	-1.0985	P3E0O...3-.	0.06788	0.484	2.2542	S3E0N...17-.	-0.86955	0.36092	-0.16061	VS3-C...14..	0.62858	-1.08268	0.37916
++++O--B2==	0.00033	-0.86163	0.35723	P3E0O...4-.	-0.76746	0.35805	-0.99768	S3E0N...2-.	-2.6125	-2.57542	-3.83907	VS3-C...15..	0.37793	0.02274	-0.84761
++++O--S===	0.37343	2.34852	0.56596	P3E0O...6-.	1.1918	0.21855	1.29067	S3E0N...18-.	0.46217	-0.52037	0.4727	VS3-C...16..	-1.31444	0.47163	-0.80138
++++S--B2==	-0.94498	0.09379	1.15443	P3E0S...0-.	-1.52955	-0.66776	-1.33533	S3E0N...22-.	0.70352	0.36249	2.36181	VS3-C...17..	0.35092	0.4005	0.03832
+.....	0.12169	2.23137	-1.46445	P3E0S...2-.	-0.60259	0.00459	0.1249	S3E0N...3-.	0.28154	0.62745	0.14374	VS3-C...18..	0.82218	-1.76164	-1.76107
+...[...(...	0.4666	-0.96084	0.17609	P3E0o...5-.	1.19429	2.4829	2.32268	S3E0N...4-.	-0.67418	-1.66158	0.31169	VS3-C...2...	0.05652	-0.84909	0.10322
-.....	0.73774	2.17354	-0.20624	P3E0s...2-.	2.2248	0.49174	0.56847	S3E0N...5-.	-1.69166	-0.71171	-1.17761	VS3-C...19..	0.6613	-0.81327	-0.93143
1...(.....	-0.65593	-0.8978	-0.65958	P3E0s...3-.	2.09169	-1.34823	-0.67445	S3E0N...6-.	0.11607	-0.50328	-2.13172	VS3-C...20..	-0.79855	0.4299	0.06104
1.....	0.23469	0.362	-0.63799	P3E0s...4-.	-0.63098	-0.76741	-0.64768	S3E0N...7-.	-1.92196	-2.48822	-2.47684	VS3-C...21..	0.0859	0.27915	-0.06633
1...C...(...	0.127	-0.86276	0.21145	P3E0s...5-.	0.02729	2.08126	-0.59206	S3E0N...8-.	6.34246	0.30649	7.34229	VS3-C...22..	0.04967	-0.69883	1.37215
1...N...(...	0.1187	-0.53176	-0.92594	P4E0C...0-.	0.03673	0.13164	-0.51676	S3E0N...9-.	0.49628	-0.96909	1.10903	VS3-C...23..	-0.1035	-0.83186	-1.66126
1...N...1...	0.03809	-0.52915	-0.76535	P4E0C...1-.	2.35265	0.46709	2.41446	S3E0O...1-.	-0.60472	0.39472	0.40726	VS3-C...24..	-0.07466	0.98817	0.95156
1...O...(...	-0.88498	0.38864	0.17417	P4E0C...10-.	-0.6321	0.39681	-0.65978	S3E0O...10-.	0.28122	0.19548	-0.44304	VS3-C...25..	-1.07451	0.17507	3.18227
1...c...(...	0.22341	-0.99896	0.61084	P4E0C...11-.	0.28657	-0.57517	-0.03405	S3E0O...11-.	0.12713	-0.71751	-0.08392	VS3-C...26..	-1.29455	0.23415	-0.49101
1...c...1...	2.31782	0.2209	2.18996	P4E0C...12-.	0.17488	0.11257	0.03593	S3E0O...13-.	0.32257	-0.22041	-0.26387	VS3-C...27..	0.36192	0.63679	0.10623
1...n...(...	-0.59508	-0.51556	-0.90082	P4E0C...13-.	0.08859	0.23814	-0.00203	S3E0O...14-.	0.11362	0.5393	-0.55909	VS3-C...3...	0.31608	-0.75248	-0.99871
1...s...(...	0.27284	-0.71909	-0.63494	P4E0C...14-.	-0.87448	0.24014	-0.51536	S3E0O...16-.	-0.89593	1.1447	-0.10181	VS3-C...28..	0.01298	2.51284	0.15574
2...(.....	-0.18978	1.20706	0.3486	P4E0C...15-.	0.08347	0.35587	2.39125	S3E0O...2-.	0.48637	-0.83209	0.3439	VS3-C...4...	-1.41126	-1.8921	-0.77316
2.....	1.16562	-0.38085	-0.02386	P4E0C...16-.	-0.14685	0.88174	2.41492	S3E0O...18-.	-0.6813	0.23235	-0.29965	VS3-C...5...	0.52259	1.21354	2.2006
2...1.....	2.43247	0.21573	0.49488	P4E0C...17-.	-1.13335	1.71664	-0.3497	S3E0O...3-.	0.19114	-0.81866	0.43117	VS3-C...6...	0.26265	0.36411	0.14558
2...C...(...	-1.29823	-0.85005	-0.4562	P4E0C...2-.	-0.59519	-0.86888	-0.07663	S3E0O...4-.	0.45776	1.17977	0.3116	VS3-C...7...	-0.20669	0.2692	-0.51665
2...C...1...	-0.34584	0.21528	5.13327	P4E0C...18-.	-0.66418	-0.1112	0.62116	S3E0O...5-.	0.32123	0.48801	-0.9824	VS3-C...8...	-0.4152	0.47601	-0.86634
2...N...(...	-0.59753	-0.64893	-0.81641	P4E0C...19-.	-0.58211	-0.97666	1.21752	S3E0O...6-.	-1.27423	-1.40484	-2.86082	VS3-C...9...	0.20062	0.39004	2.30174
2...c...(...	0.23214	1.48488	0.21828	P4E0C...20-.	0.54085	0.13455	-0.7605	S3E0O...7-.	0.06591	0.32265	0.17748	VS3-F...12..	0.07601	0.06354	1.3288
2...c...1...	0.29629	2.34635	0.27389	P4E0C...21-.	-0.47214	-0.59699	-0.90846	S3E0O...8-.	-1.09061	-0.46665	0.59154	VS3-F...14..	-0.64664	0.22239	0.54655
2...n...(...	-0.08498	0.44589	1.0796	P4E0C...22-.	0.79902	0.48087	-0.58937	S3E0O...9-.	0.46003	0.21198	0.05187	VS3-F...4...	-0.03069	-0.7939	2.03155
2...n...1...	-0.31951	-0.5852	-0.03401	P4E0C...3-.	-0.85977	0.08411	-0.12165	S3E0S...0-.	2.46055	2.39138	4.0295	VS3-F...5...	0.32291	0.00493	0.0225
2...s...(...	3.22974	-0.99767	0.42339	P4E0C...4-.	0.37249	0.21562	0.11033	S3E0S...1-.	0.42681	-0.65865	-0.54173	VS3-F...8...	-0.48159	0.1574	-0.43043
3...(.....	-0.35933	0.4267	-1.25771	P4E0C...5-.	-0.07252	0.66654	0.00024	S3E0S...2-.	-0.04621	0.40626	2.20527	VS3-F...9...	-0.70097	0.36599	-0.14776
3.....	0.17567	0.1593	-0.76906	P4E0C...6-.	-0.51102	0.391	-0.79997	S3E0S...4-.	-0.59783	-0.53875	-1.25536	VS3-Br...6...	0.13112	-0.52139	-0.07933

3...2.....	-0.21245	0.08535	-0.32244	P4E0C...7-..	0.06986	2.21851	1.03921	S3E0o...12-.	0.21274	0.00753	2.3293	VS3-Cl..4...	0.35633	0.28498	2.46617
3...C...(...	-0.83079	-0.64525	-0.21388	P4E0C...8-..	0.20582	2.17532	0.11798	S3E0s...10-.	-0.75985	0.44265	2.19473	VS3-Cl..5...	-0.60661	-0.45445	-1.3015
3...N...(...	0.16106	-0.06718	0.62235	P4E0C...9-..	-0.84545	-0.74308	-0.55846	S3E0s...11-.	-2.48499	-1.12857	-0.46342	VS3-Cl..6...	-0.78819	2.11069	2.30181
3...c...(...	1.29651	0.05486	0.46129	P4E0F...1-..	1.40265	-1.03377	1.89129	S3E0s...12-.	0.28428	2.07933	2.05072	VS3-Cl..7...	0.39618	0.38194	2.1227
3...c...1...	-0.96535	-0.88711	-0.60174	P4E0F...16-.	-0.50121	-0.58235	-0.75328	S3E0s...13-.	0.11451	0.17937	0.28619	VS3-Cl..8...	2.49663	0.26102	2.19678
3...c...2...	0.30449	-0.71089	0.43858	P4E0F...3-..	0.60456	0.38711	-0.72464	S3E0s...7-..	-0.85254	-0.80958	0.07899	VS3-N...10..	0.02307	0.24638	0.26086
3...n...(...	0.95222	-0.33623	0.14716	P4E0F...4-..	0.24386	1.23133	-0.68921	S3E0s...8-..	-0.07345	-0.37262	0.17506	VS3-N...11..	3.69483	-0.74784	-0.22654
=...(.....	0.02402	-0.13964	-0.8594	P4E0F...7-..	0.38579	-0.72426	-0.93929	S3E0s...9-..	-0.90968	-1.43268	-0.19128	VS3-N...12..	2.2463	0.42839	2.45604
=...(.....	0.13294	-0.84407	0.49496	P4E0Br...7-..	-0.66169	-0.14103	0.03667	PT2-C...1...	0.48657	0.38133	0.13775	VS3-N...13..	0.28577	-0.64961	-0.54677
=.....	-0.55327	0.18729	-0.67134	P4E0Cl...1-..	0.67112	2.23465	0.73008	PT2-C...2...	0.09296	-0.63839	-0.14644	VS3-N...14..	0.36009	0.04591	0.45642
=...1.....	2.24897	0.49522	0.30898	P4E0Cl...3-..	2.23396	2.15129	0.81639	PT2-C...3...	0.21322	-0.29998	0.39689	VS3-N...15..	-1.11397	0.25048	-1.05666
=...2.....	0.32882	-0.85663	0.05474	P4E0Cl...4-..	-0.66806	-0.74482	0.77829	PT2-C...4...	0.11839	-0.81438	-0.92069	VS3-N...16..	0.07843	0.24677	-0.87514
=...C...(...	0.58574	-0.65692	-0.67769	P4E0N...0-..	-0.00489	-0.54044	-0.67426	PT2-C...5...	-0.75292	0.12187	-0.87179	VS3-N...18..	0.25064	-0.85874	2.21563
=...C...1...	0.23079	-0.11838	2.45331	P4E0N...1-..	0.39622	0.73037	-0.95318	PT2-C...6...	0.28327	1.38791	0.37658	VS3-N...20..	3.39642	0.07714	-0.17803
=...N...(...	-0.61832	0.05467	-0.66972	P4E0N...10-.	2.83833	1.79948	5.54355	PT2-C...7...	0.37711	-0.55212	0.21182	VS3-N...21..	0.34204	-0.64353	0.56463
=...O...(...	0.41795	0.34936	-0.56761	P4E0N...11-.	-0.54287	0.46522	-0.77217	PT2-F...2...	0.09445	0.65438	1.9631	VS3-N...25..	-0.6302	-0.51561	-1.08392
=...S...(...	0.35368	-0.6422	-0.73137	P4E0N...12-.	0.00583	1.38921	-0.8959	PT2-F...3...	0.06839	-0.4041	0.00227	VS3-N...3...	-0.66262	-0.31113	-0.7804
=...c...1...	0.35866	0.48515	-0.97424	P4E0N...13-.	4.42962	1.72127	3.26743	PT2-Br...2...	0.14258	0.04525	2.08006	VS3-N...4...	0.22084	0.07795	-0.71844
C...(.....	0.0426	-0.67721	0.17864	P4E0N...15-.	-0.51528	0.4271	-0.7184	PT2-Cl...2...	-0.14086	-0.21292	1.84524	VS3-N...5...	-0.62385	0.06777	-1.77256
C...(.....	-0.71913	0.2184	-0.533	P4E0N...16-.	-0.57215	0.0389	-0.55366	PT2-Cl...3...	0.20608	0.22394	0.1782	VS3-N...6...	-1.8578	-1.57997	-1.39506
C...(.....1...	0.39929	0.062	0.46727	P4E0N...2-..	0.31935	-0.84497	0.39233	PT2-N...1...	-0.12615	-0.77577	0.45566	VS3-N...7...	0.05164	1.89836	2.05437
C...(.....2...	0.27037	0.44539	2.20457	P4E0N...21-.	1.35126	-0.09036	0.04584	PT2-N...2...	0.34689	0.42706	0.18482	VS3-N...8...	-0.01223	0.86589	-1.47814
C...(.....3...	1.14044	1.9098	2.71117	P4E0N...3-..	0.15786	0.14991	0.0797	PT2-N...3...	0.20475	-0.65931	0.28685	VS3-N...9...	0.07745	0.28184	0.1021
C...(.....=...	0.381	0.43397	-0.28917	P4E0N...4-..	0.49062	-0.66291	0.5915	PT2-N...4...	0.28305	0.16108	0.19124	VS3-O...10..	1.14408	0.015	-0.85979
C...(.....C...	-0.36795	-0.8476	-0.88639	P4E0N...5-..	-0.77823	0.07997	0.23926	PT2-N...5...	-1.64622	0.98206	-3.36207	VS3-O...11..	-0.55834	-0.13345	0.36688
C.....	0.36029	0.4981	0.10225	P4E0N...6-..	0.37231	-0.08637	-0.22597	PT2-N...6...	0.12406	0.15404	0.69576	VS3-O...12..	-0.38988	0.38124	0.35929
C...1...(...	0.01491	-0.85259	0.65863	P4E0N...7-..	-0.86138	0.04756	-0.41231	PT2-O...1...	0.0989	0.27965	-0.82726	VS3-O...14..	0.27115	-0.68045	0.17811
C...1.....	0.12928	-0.51331	-0.60892	P4E0N...8-..	-0.51269	-0.50521	-1.96934	PT2-O...2...	-0.95839	0.26055	0.73401	VS3-O...16..	-0.83577	-1.13391	-0.83799
C...1...2...	-0.07439	-1.73339	-0.93486	P4E0N...9-..	-0.81125	0.19782	-0.74658	PT2-O...3...	0.14522	-0.77756	0.07567	VS3-O...18..	0.29996	-0.53936	0.28477
C...1...=...	0.69187	-0.71348	0.74685	P4E0O...0-..	0.05774	0.03625	0.21987	PT2-O...4...	0.4542	2.18124	0.36764	VS3-O...2...	-1.80306	-0.93739	-2.32978
C...1...C...	0.00808	-0.07592	-0.54204	P4E0O...1-..	-0.92106	-0.87576	-3.1221	PT2-O...5...	-0.67123	0.23542	1.92304	VS3-O...20..	-0.53141	-0.51742	-0.05428
C...2...(...	-0.82253	0.53996	-1.99396	P4E0O...10-.	1.37399	1.23763	0.14762	PT2-S...2...	0.21616	0.40146	0.46449	VS3-O...3...	0.06582	-0.9475	0.12857
C...2.....	-0.85598	0.25635	-0.90303	P4E0O...12-.	0.3884	-1.03888	-0.97448	PT2-S...3...	0.59137	-0.02005	-0.54081	VS3-O...4...	1.14146	0.42055	-0.49425
C...2...1...	0.07476	-0.68238	0.10291	P4E0O...14-.	-0.3666	-0.57548	-0.69097	PT2-o...4...	-1.11608	0.85916	1.37411	VS3-O...5...	4.22681	4.43798	5.08434
C...2...=...	0.48881	0.22294	0.16378	P4E0O...16-.	1.14479	0.34688	1.28314	PT2-s...3...	0.42042	-0.19048	-1.39227	VS3-O...6...	-0.34913	-0.89338	-0.65311

C...2...C...	1.28778	1.48801	1.34452	P4E0O...3-..	-0.06635	0.24579	0.19778	PT2-s...4...	0.1687	-0.80481	-0.04818	VS3-O...7...	-1.09665	-0.08502	-0.79459
C...3.....	-0.14854	0.60233	-0.70534	P4E0O...4-..	-1.76903	-0.97362	-1.21244	PT3-C...1...	-0.00361	-0.29636	0.42818	VS3-O...8...	0.17318	0.20809	0.40586
C...3...2...	0.43343	0.05177	0.34101	P4E0O...6-..	-0.93073	0.55068	0.37658	PT3-C...10..	0.40598	0.27364	0.0772	VS3-O...9...	0.1522	0.09551	2.08664
C...3...C...	-0.97337	-0.83717	0.30997	P4E0O...7-..	0.06521	-0.88499	0.13988	PT3-C...11..	0.38211	2.17648	0.42649	VS3-S...4...	2.71307	0.42803	2.23117
C...=.....	0.19828	2.29894	0.73351	P4E0O...8-..	0.0463	0.05354	2.22939	PT3-C...2...	0.30851	1.5748	2.98965	VS3-S...5...	0.49147	0.3805	-0.66051
C...=...2...	-0.84171	0.1843	-1.11049	P4E0O...9-..	0.31702	0.09603	0.02066	PT3-C...3...	-0.07117	0.08367	0.11721	VS3-S...6...	0.37594	0.16978	2.03871
C...=...C...	0.05868	2.05932	2.22431	P4E0S...2-..	1.06393	0.13586	0.39549	PT3-C...4...	-0.67029	0.05381	-0.79483	VS3-S...8...	-0.6482	-1.07329	-0.91176
C...C...(...	-0.51832	-0.77962	-1.22996	P4E0o...11-	2.16592	0.21668	-0.12701	PT3-C...5...	-0.34693	0.29252	0.10255	VS3-o...14..	1.51645	0.53745	0.60259
C...C.....	0.19676	0.08445	2.04398	P4E0s...10-	0.4324	0.03005	-0.91068	PT3-C...6...	2.82453	2.50315	0.16137	VS3-s...10..	0.72899	-0.27296	1.61405
C...C...1...	-0.97671	0.33139	-0.8968	P4E0s...12-	-0.79883	-0.08105	-0.4817	PT3-C...7...	0.28934	0.31924	0.48458	VS3-s...11..	-0.71413	0.31911	-1.41887
C...C...2...	-0.16842	0.24163	-0.01064	P4E0s...13-	-0.69294	1.4305	0.59251	PT3-C...8...	-0.68656	0.10179	-0.84464	VS3-s...12..	0.09605	0.46761	2.14086
C...C...3...	-0.77175	-0.55131	-0.91806	P4E0s...4-..	0.63412	1.22253	2.30469	PT3-C...9...	0.42159	0.28775	0.10701	VS3-s...13..	-2.39683	-0.27375	-0.81188
C...C...=...	-0.11563	2.35786	2.08774	P4E0s...7-..	0.26272	-0.0982	-0.96587	PT3-F...2...	0.36062	0.06053	2.18872	VS3-s...14..	0.84408	0.8975	4.351
C...C...C...	-0.2775	2.4566	0.19253	NNC-C...101.	1.40151	-0.87039	2.00634	PT3-F...3...	-0.68204	0.0066	0.49534	VS3-s...15..	0.15259	0.09006	-0.87313
C...N...(...	-0.86866	-0.81376	-0.82108	NNC-C...110.	0.39099	0.38621	0.10264	PT3-F...4...	0.24129	0.40447	0.48843	VS3-s...9...	-0.86286	0.36693	0.14742
C...N...1...	2.15353	0.16584	0.89351	NNC-C...202.	0.22192	2.11251	1.13826	PT3-F...7...	0.97073	-0.51039	-0.47292	Smax.0.....	2.49398	-0.92216	-0.46067
C...N...3...	1.14364	0.17982	2.37754	NNC-C...211.	0.04875	0.43672	0.22454	PT3-Br...4...	-0.73756	-0.68119	0.49614	Smax.1.....	2.49694	2.32076	0.64499
C...N...=...	1.17796	2.02355	-0.94388	NNC-C...220.	-0.38888	0.17749	2.28157	PT3-Cl...2...	2.09088	0.14736	0.02322	Smax.2.....	-0.78477	-0.75287	-0.68845
C...N...C...	0.14993	-0.91813	-0.89699	NNC-C...303.	0.67268	-0.11969	0.35905	PT3-Cl...3...	-0.96086	2.36389	1.58977	[...(...	0.64432	0.10506	1.50911
C...O...(...	0.08645	0.17415	2.33068	NNC-C...312.	-0.77168	0.2155	0.03874	PT3-N...1...	0.73689	0.48545	0.31009	[...(...	0.0648	0.6247	2.73281
C...O...1...	-0.18786	0.02541	2.28111	NNC-C...321.	-1.87379	-1.38289	-1.93388	PT3-N...2...	-1.0877	-1.00831	-0.65871	[...+.....	-0.11551	-0.0844	-0.10383
C...O...2...	0.21609	-0.1634	2.10102	NNC-C...330.	0.07436	2.27038	0.31491	PT3-N...3...	0.05121	0.25525	-0.00146	[...+...N...	2.3384	0.46895	-1.30753
C...O...C...	2.34818	0.32628	0.15414	NNC-C...404.	0.20574	2.47555	-0.03329	PT3-N...4...	1.41201	0.11992	-1.04535	[...-.....	1.4791	0.29206	2.56089
C...c...1...	0.13825	2.36363	2.26321	NNC-C...431.	-0.05027	0.11701	0.50682	PT3-N...5...	0.0364	0.37208	-0.90778	[...-...O...	1.5083	-0.95009	0.18294
C...c...2...	2.36203	-0.05159	2.36611	NNC-C...440.	0.25914	-0.98302	0.42725	PT3-N...6...	-1.59339	0.17857	-0.47615	[.....	0.00771	-2.72871	-0.98249
C...n...1...	0.22413	0.12942	0.28199	NNC-F...110.	-0.72522	0.36455	-0.0277	PT3-N...7...	-0.9801	-0.29528	0.34496	[...2...(...	-0.83391	0.63213	2.39159
C3.....0...	0.25687	2.52917	-5.69739	NNC-Br...101.	-1.24166	0.79157	-0.67207	PT3-N...8...	0.11578	1.02792	0.72699	[...2.....	0.01313	-1.05297	-1.21786
C3.....1...	5.3122	-1.32744	5.39159	NNC-Cl...110.	0.78342	-4.3267	-3.13984	PT3-N...9...	0.04053	0.00452	2.31339	[...H.....	0.60809	-0.54418	0.84679
C4.....0...	10.9495	5.28164	3.93305	NNC-N...101.	0.27258	0.31054	-0.14835	PT3-O...1...	-0.57906	-1.03822	-0.4553	[...N...+...	0.20384	2.14627	-0.70111
C5.....0...	0.2976	-0.62016	0.35106	NNC-N...110.	0.0993	-0.06403	-0.66328	PT3-O...2...	0.23218	0.23841	0.56082	[...N.....	0.04474	1.26872	-1.13079
C5.....1...	2.1364	2.36404	0.41622	NNC-N...202.	2.38553	2.22296	0.01698	PT3-O...3...	-1.03701	-2.02252	-1.04855	[...O...-...	0.37919	-0.5535	-0.61776
C5....H.1...	-1.22659	0.08819	2.56134	NNC-N...211.	-1.23216	-0.00042	-0.69167	PT3-O...4...	2.49154	1.55484	-1.43594	[...O.....	0.45351	0.05236	2.38921
C5...AH.1...	2.18105	2.08893	-0.96514	NNC-N...220.	-0.54997	0.16589	0.17591	PT3-O...5...	-0.53431	0.44448	-0.71848	[...[...-...	-0.33568	0.05807	-1.44435
C5...AH.2...	0.12012	-0.06178	0.41046	NNC-N...312.	-0.78718	0.28003	2.25449	PT3-O...6...	-0.61391	-0.77592	0.65364	[...[.....	0.31865	2.25042	1.28382
C6.....0...	-0.86584	0.01087	0.02474	NNC-N...321.	0.03396	0.02931	-0.81699	PT3-O...7...	0.94745	-0.5103	-0.94878	[...[...N...	0.34085	0.24628	0.21973

C6.....3...	0.49362	-0.9465	-0.40822	NNC-N...330.	0.34683	-0.18532	-0.55508	PT3-O...8...	1.39304	2.45949	1.57125	[...n...H...	0.17819	0.21443	-0.74039
C6...A...1...	0.24721	0.00476	2.11708	NNC-O...101.	0.03696	2.3721	0.27363	PT3-S...2...	0.0158	2.12671	0.53822	c...(...(...	-0.80362	0.23616	-0.64241
C6...A...2...	0.1761	-0.53812	2.35701	NNC-O...110.	-0.5627	-0.46672	-0.79118	PT3-S...4...	-0.58552	-0.95471	-1.17046	c...(.....	-0.69573	0.00462	-0.34324
C6...AH.2...	2.12902	2.24972	1.76498	NNC-O...220.	2.43317	-0.62382	-0.46884	PT3-o...7...	0.14302	0.04176	1.41378	c...(...1...	-0.40574	2.00683	2.42012
C6...AH.3...	-0.09673	0.60009	-0.72518	NNC-S...413.	0.5776	0.31771	0.07894	PT3-s...4...	1.32552	0.45803	0.15986	c...(...2...	0.3742	-0.79583	0.2262
C6...AH.4...	2.15532	0.35562	-0.23698	NNC-o...220.	0.33933	0.23206	2.30898	PT3-s...5...	-0.53378	-0.04039	0.10905	c...(...3...	0.41437	0.45747	0.23251
C6...AH.5...	-0.96303	-0.847	2.10138	NNC-s...211.	0.01686	-0.74096	-0.03189	PT3-s...6...	0.05067	0.26133	0.15798	c...(=...=...	-0.74187	0.01276	0.00833
C7.....0...	0.02773	-0.77968	0.28712	NNC-s...220.	0.49316	0.01282	0.49778	PT3-s...7...	2.13173	2.305	1.40865	c...(...C...	0.54077	0.13723	0.32186
C7....H.2...	1.63121	0.26826	0.15418	NNEOC...100-	0.46875	0.1526	0.01442	PT4-C...1...	0.48246	-0.71371	0.10312	c...(...F...	-0.96525	-0.35509	0.25094
C7...AH.1...	0.40307	1.23492	0.59142	NNEOC...109-	0.51133	0.44263	1.19882	PT4-C...10..	0.11613	-0.94589	0.41149	c...(...Cl...	2.30634	0.58646	0.18212
BOND00000000	1.7243	1.78708	-0.03511	NNEOC...200-	-0.35737	0.37196	0.14582	PT4-C...11..	0.02384	0.45068	-0.59787	c...(...N...	-0.69498	0.05861	0.08447
BOND10000000	1.39454	2.09746	0.23456	NNEOC...209-	-0.8685	0.30216	0.3322	PT4-C...12..	0.26511	0.03568	0.67452	c...(...O...	0.09724	0.14	1.11846
F...(...(...	1.58952	1.4189	2.03016	NNEOC...218-	0.23108	0.04018	2.49076	PT4-C...13..	0.42191	-0.2398	0.58849	c...(...c...	-0.19484	-0.96251	-0.45733
F...(.....	-0.8507	-0.0577	-0.95708	NNEOC...300-	-0.10743	-0.3502	-0.81493	PT4-C...14..	0.26987	0.02317	0.49044	c.....	0.3234	0.22145	0.27649
F...(...2...	-0.95236	-0.85601	-0.79635	NNEOC...309-	0.47999	0.35377	-0.90649	PT4-C...15..	0.41204	0.26793	0.69911	c...1...(...	-0.80762	-0.99285	-1.51468
F...(...C...	0.13756	-0.04046	-1.48119	NNEOC...318-	-1.12389	-0.76577	-1.16172	PT4-C...16..	-0.31343	1.12137	0.46747	c...1.....	-0.84576	-0.70789	2.24097
F...(...F...	0.09098	1.11525	2.03365	NNEOC...327-	0.44857	-0.02887	-0.71884	PT4-C...17..	0.36354	0.27954	0.24983	c...1...C...	0.16739	0.30507	0.20554
F.....	1.152	0.24746	0.19111	NNEOC...400-	2.24693	0.51396	2.23893	PT4-C...2...	0.17442	0.33558	2.16342	c...1...N...	0.36159	0.04854	0.10081
F...c...1...	-0.09728	0.0051	-0.70931	NNEOC...427-	0.15258	-0.49998	0.27901	PT4-C...18..	-0.07622	0.43944	0.23218	c...1...O...	0.05096	0.45434	0.20975
EC0-C...1...	0.1531	-0.24547	-0.77845	NNEOC...436-	2.23904	-0.95356	-0.51509	PT4-C...19..	0.38463	0.06249	1.85676	c...1...c...	0.13001	0.10652	-0.20118
EC0-C...2...	2.23296	0.25736	2.13228	NNEOF...109-	-0.6351	-0.69949	0.46634	PT4-C...20..	2.3714	0.01694	2.47522	c...2...(...	0.05797	0.27429	-0.78645
EC0-C...3...	-0.63312	-0.7726	-0.47091	NNE0Br...100-	-0.96941	-0.11348	-0.86235	PT4-C...21..	0.01636	0.23208	-0.247	c...2.....	0.48584	-0.07836	2.02182
EC0-C...4...	-1.8154	-0.81627	1.83731	NNE0Cl...109-	0.18372	0.17389	2.19206	PT4-C...22..	-0.23446	0.13119	0.48307	c...2...=...	0.25379	0.30424	0.22695
EC0-F...1...	0.38793	-0.73916	0.32177	NNE0N...100-	-0.80318	-0.45752	0.28021	PT4-C...24..	0.26973	-0.53965	-0.09164	c...2...Cl...	2.11886	2.48767	2.36215
EC0-Br...1...	-0.34958	-0.80174	-0.90168	NNE0N...109-	-0.83559	0.35455	0.0206	PT4-C...25..	2.17928	-0.12469	-0.74503	c...2...c...	1.40592	1.55829	2.05199
EC0-Cl...1...	0.26043	2.23316	2.21212	NNE0N...200-	1.34899	2.28282	2.43439	PT4-C...3...	1.99214	2.40479	-0.56618	c...3...(...	0.06076	0.90611	-0.6936
EC0-N...1...	0.49324	-0.87888	0.40049	NNE0N...209-	0.009	0.39312	-0.85573	PT4-C...4...	1.13933	0.03684	2.2256	c...3.....	-0.06552	-0.9892	0.08731
EC0-N...2...	-0.52908	0.40746	0.18437	NNE0N...218-	0.02276	0.52399	2.13104	PT4-C...5...	-1.04995	-0.61142	-2.61617	c...3...c...	-0.55897	0.07795	0.06945
EC0-N...3...	-1.01916	-0.03247	1.79208	NNE0N...309-	1.55866	-0.1332	-0.37739	PT4-C...6...	1.39341	0.27457	-0.05959	c...=.....	0.2537	0.47788	0.49889
EC0-O...1...	-0.92155	-0.67765	-0.87997	NNE0N...318-	-0.18673	-0.80153	-0.06489	PT4-C...7...	0.17292	1.06074	0.26559	c...=...N...	0.19769	-0.66864	0.27929
EC0-O...2...	-0.86981	0.22862	2.35716	NNE0N...327-	0.28417	0.15478	0.43525	PT4-C...8...	0.29601	0.30338	-0.60323	c...C...(...	-0.23827	2.01716	1.68518
EC0-S...4...	1.06947	-0.79758	0.1354	NNE0O...100-	0.4907	0.19715	0.08214	PT4-C...9...	2.00248	0.4119	2.68775	c...C.....	2.22333	0.36062	2.05477
EC0-o...2...	2.13513	0.3829	2.45378	NNE0O...109-	-0.59596	-1.18051	-0.58622	PT4-F...17..	0.16264	-0.94288	-0.88286	c...C...1...	0.12218	-0.22607	-0.2383
EC0-s...2...	-0.01819	0.43769	-0.06105	NNE0O...218-	-0.98042	0.13465	2.14414	PT4-F...2...	-0.85722	-0.96742	0.07513	c...C...C...	0.06055	-0.31014	0.44015
H.....	0.23229	-0.0546	0.28908	NNE0S...409-	0.43544	-0.38037	-0.88913	PT4-F...4...	-0.35181	2.13037	-0.23636	c...F.....	0.34773	-0.88323	-0.74301

H...[...2...	-1.86843	-0.10128	1.69945	NNE0o...218-	2.40415	1.58007	2.17219	PT4-F...5...	0.23527	-0.94556	0.02251	c...Cl.....	0.3638	0.98209	0.46919
Br..(.....	0.48079	-1.18479	-0.22349	NNE0s...209-	-0.26647	0.77009	-0.93241	PT4-F...8...	0.27782	1.1436	0.54611	c...N...(...	-1.01708	0.13434	0.13576
Br.....	-1.29212	-0.96051	-0.08624	NNE0s...218-	0.48799	-0.92109	0.08824	PT4-Br..8...	-0.68945	-0.44919	0.39977	c...N.....	-1.11674	-0.34213	-0.61079
Cl..(...(...	0.12882	-0.05669	2.00894	NOSP01000000	0.69355	2.2604	3.67548	PT4-Cl..2...	2.77031	0.69825	0.29226	c...N...=...	-0.89514	0.57778	2.48047
Cl..(.....	-0.76812	2.19447	0.02542	NOSP10000000	-3.86395	-2.32737	-3.57245	PT4-Cl..4...	0.17285	0.187	-0.19396	c...O...(...	-0.68651	0.30096	0.09369
Cl..(..1...	2.56646	0.09187	0.58522	NOSP11000000	-0.96156	0.05503	0.43511	PT4-Cl..5...	1.01445	-0.8606	1.32509	c...O.....	-4.4891	-1.77794	-4.57051
Cl..(..C...	-0.19283	0.81579	-1.08229	NOSP11100000	0.25443	-0.61999	-0.56449	PT4-N...1...	-0.74846	0.11784	-0.40604	c...O...C...	-0.35817	0.07334	-0.75285
Cl..(..Cl..	2.1219	0.35966	2.06911	S...(.....	0.03	0.15688	0.11096	PT4-N...10..	-0.93246	0.23828	0.35363	c...[.....	2.10877	-0.11899	0.15261
Cl.....	2.24905	2.23591	0.45911	S...(..1...	0.28735	-0.2473	-0.98364	PT4-N...11..	-1.31385	0.7013	-0.62835	c...c...(...	0.18143	0.47407	-0.74955
Cl..2.....	2.24474	0.64454	0.24622	S...(..2...	-0.85261	-0.41388	0.02192	PT4-N...12..	1.43096	-0.73105	-0.07674	c...c.....	0.29466	0.00755	0.21636
Cl..c...1...	2.43857	1.88477	2.1353	S...(..=...	0.45053	0.00647	0.49728	PT4-N...13..	-0.92395	0.36236	0.19211	c...c...1...	-0.73075	1.40562	-0.5987
Cmax.1.....	3.96897	1.5883	2.43778	S...(..C...	-0.99744	0.28391	0.3741	PT4-N...14..	0.35328	-0.31741	-0.69679	c...c...2...	2.10322	2.04984	-0.6361
Cmax.2.....	2.04493	0.49477	2.32662	S...(..F...	-0.31012	0.14915	-0.09756	PT4-N...15..	0.60607	1.21863	2.15923	c...c...3...	0.42177	0.22771	-0.04625
Cmax.3.....	-0.81812	0.15524	-1.00546	S...(..Cl..	-0.98941	0.35685	2.19665	PT4-N...16..	-0.00847	0.28332	0.49334	c...c...[...	-0.60049	0.18941	0.45452
HALO00000000	-0.7146	-0.05095	2.02724	S.....	-0.54618	0.28476	-0.1144	PT4-N...2...	-0.28191	-0.08045	0.03124	c...c...c...	2.38658	2.03972	-0.14827
HALO00100000	0.30447	0.29506	-0.74387	S...=.....	-0.76276	-0.59939	-1.74529	PT4-N...18..	-0.5553	0.01363	1.20508	c...n...1...	2.34275	-0.05757	-0.85846
HALO01000000	0.31657	1.4348	2.24296	S...=...O...	-0.58871	-0.72443	-0.76909	PT4-N...23..	0.17981	0.04282	2.04369	c...n...2...	0.0567	-0.65144	0.42208
HALO10000000	0.15215	0.50422	0.19177	S...N.....	4.04473	2.57595	2.27636	PT4-N...3...	-1.54905	-0.92011	-1.99161	c...n...c...	0.50033	-0.09799	-0.73447
N...(.....	-0.98213	-0.43118	-0.74526	S...N...C...	2.00984	2.17684	2.40769	PT4-N...4...	0.16895	-0.58029	0.92841	c...o...1...	0.58602	0.33237	2.46204
N...(..1...	-0.73573	0.19138	-1.66626	S2E0C...0-..	-0.73359	-0.5248	0.19216	PT4-N...5...	0.48893	0.04423	0.14851	c...s...(...	1.41242	2.42007	2.14644
N...(..C...	-0.16151	-0.69959	-1.11224	S2E0C...1-..	2.15113	0.2877	1.97429	PT4-N...6...	-0.72108	-0.80907	-1.54523	c...s...1...	-0.13541	-0.86024	-0.87466
N...(..Br..	-0.71201	-0.17824	-0.89366	S2E0C...10-.	0.49906	-0.78935	0.32473	PT4-N...7...	-0.75736	0.26704	-0.72268	n...(.....	0.28813	-0.77834	0.46756
N...(..Cl..	-1.10752	-1.23234	-0.69452	S2E0C...11-.	-0.28542	0.12827	-0.60342	PT4-N...8...	0.19611	0.16111	-0.62782	n...(..1...	0.06525	-0.59211	0.29214
N...+.....	3.16015	-0.51411	-0.5429	S2E0C...12-.	0.89961	0.38099	-0.30088	PT4-N...9...	0.2813	0.4231	0.23066	n...(..C...	0.16693	-0.88399	0.28242
N.....	-0.54824	-0.63407	-0.58104	S2E0C...13-.	0.12725	-0.06893	0.26187	PT4-O...1...	0.26183	-0.92006	-0.69661	n...(..c...	0.00941	0.01508	0.46693
N...1.....	0.8894	0.42028	0.35541	S2E0C...14-.	-0.00453	-0.37356	1.42629	PT4-O...10..	2.35144	0.21096	-0.0059	n.....	0.4575	0.17876	-0.17955
N...1...C...	-0.79109	0.0528	0.09087	S2E0C...2-..	0.32428	-0.58822	-0.5034	PT4-O...12..	0.08583	-0.17191	-1.36991	n...1.....	-0.94463	0.05721	-0.60436
N...2.....	-0.84924	-0.60611	-0.65611	S2E0C...3-..	0.40489	0.19081	-0.67242	PT4-O...13..	0.2836	0.3599	-0.79216	n...1...C...	0.28986	0.2403	0.41335
N...2...C...	-0.73041	-0.98743	0.88434	S2E0C...4-..	0.27431	0.1603	-0.64726	PT4-O...16..	0.1205	2.46834	-0.76365	n...1...c...	0.04809	0.2972	0.44477
N...3...(...	-0.63823	0.34296	-0.52578	S2E0C...5-..	0.37647	2.01944	0.26899	PT4-O...17..	0.33138	0.35309	0.14275	n...1...n...	0.20482	-0.46933	-0.76917
N...3.....	0.46444	-0.63348	0.38401	S2E0C...6-..	0.42791	0.60321	2.36668	PT4-O...2...	0.4262	0.01935	-0.3871	n...2...(...	1.78882	0.14691	-0.96149
N...3...C...	-0.68855	-0.96999	-0.09593	S2E0C...7-..	0.7445	-0.06783	0.09719	PT4-O...3...	-0.16899	-0.62538	-2.83432	n...2.....	0.81075	2.38662	-0.49785
N...=.....	-0.58571	0.30395	-0.77591	S2E0C...8-..	2.05445	0.47146	1.27482	PT4-O...4...	0.13171	-0.05053	-0.53118	n...2...c...	-1.43426	-0.74927	-0.98687
N...=...1...	0.01826	0.47723	2.07009	S2E0C...9-..	0.72539	-0.84867	0.64405	PT4-O...5...	-0.43913	-0.75735	-1.97766	n...3.....	0.1576	-0.26927	0.25977
N...=...2...	-0.91192	2.47375	-0.9808	S2E0F...3-..	-0.09403	2.09555	2.43903	PT4-O...6...	2.14377	0.22792	-0.5518	n...3...c...	-1.81039	-0.81147	-0.65304

N...C...(...	0.01411	0.41735	2.44216	S2E0F...4-..	-0.42171	-0.53968	1.22683	PT4-O...8...	0.6644	0.29318	2.36116	n...C.....	1.02189	-0.97424	-0.93995
N...C.....	0.18303	-0.75833	-0.54585	S2E0F...5-..	-0.68133	0.56812	-0.70322	PT4-O...9...	0.34854	0.29352	-0.88037	n...C...C...	-0.82773	0.17539	0.09117
N...C...1...	1.18224	1.15252	0.11132	S2E0F...9-..	-0.45558	-0.74241	0.6498	PT4-S...2...	0.13977	0.34717	0.338	n...H.....	0.15952	-0.63695	0.00967
N...C...C...	-0.99504	0.30907	-0.76519	S2E0Br...5-..	-0.30676	0.24666	-0.40556	PT4-S...6...	-1.18884	0.19	-1.86095	n...H...[...	2.02601	-0.94357	1.70404
N...S...(...	1.76899	2.61791	2.63934	S2E0Cl...3-..	1.31385	1.19854	2.0981	PT4-o...13..	2.35863	0.19809	0.77903	n...[.....	0.05557	-1.09898	0.37211
N...c...1...	-1.32191	0.12661	-0.8796	S2E0Cl...4-..	-0.78187	-1.52933	1.5693	PT4-s...12..	0.17607	-0.93961	-0.06524	n...[...c...	-0.14457	-0.92874	-1.10231
O...(...	-0.52341	0.26602	2.29637	S2E0N...1-..	0.25085	2.15343	0.04602	PT4-s...14..	0.25166	0.27855	0.03999	n...c...(...	-0.82798	-0.61881	0.06095
O...(.....	-0.52586	-0.39601	-0.63779	S2E0N...10-..	-1.21878	-0.80358	0.33984	PT4-s...15..	-0.08379	0.02761	-0.968	n...c.....	-0.55416	0.01662	1.9503
O...(...1...	0.48508	-1.32985	-0.71987	S2E0N...11-..	0.15357	0.11468	2.33164	PT4-s...6...	0.49943	0.03813	2.43373	n...c...1...	1.25184	0.32134	2.17753
O...(...2...	0.2826	0.14065	-0.55389	S2E0N...2-..	0.29108	-0.63473	-0.27501	PT4-s...9...	0.2372	-0.32296	-0.46931	n...c...2...	0.32311	0.18498	0.58804
O...(...C...	-0.51582	-0.98786	-0.5871	S2E0N...3-..	0.15907	0.18969	2.03791	Nmax.0.....	-0.9234	1.38661	0.04236	n...c...c...	0.41251	-0.78184	2.08239
O...(...N...	-0.81738	-0.99472	-0.69132	S2E0N...4-..	1.05339	1.54638	-0.66466	Nmax.1.....	1.38641	0.41952	-0.75135	n...c...n...	-0.66901	0.32885	3.42654
O...(...O...	0.46016	0.11023	1.33529	S2E0N...5-..	1.12581	2.20028	-0.98431	Nmax.2.....	-0.12645	-0.7017	-0.75869	n...n...(...	-0.72211	2.71273	0.29177
O...-.....	0.16235	-0.85863	0.44675	S2E0N...6-..	0.03234	0.12178	0.1397	Nmax.3.....	0.67479	-0.44966	0.07735	n...n.....	-0.54765	0.43715	2.0837
O.....	-1.25961	-0.32181	-0.55125	S2E0N...7-..	-2.51138	-1.0895	-0.23354	Nmax.4.....	-0.56908	-0.57795	-0.77003	n...n...1...	0.3625	-0.51506	-0.44598
O...1.....	-0.45431	0.71467	-0.76434	S2E0N...8-..	-0.97985	0.09852	-0.99536	Omax.0.....	-0.2616	0.25178	-0.74982	n...n...2...	0.74054	-0.08303	2.47641
O...1...C...	-0.73726	-0.82182	2.26821	S2E0N...9-..	-0.83898	2.14709	0.17445	Omax.1.....	0.48225	-0.09916	-0.81615	n...n...c...	0.48285	-0.99433	0.24124
O...2.....	-0.75627	-0.0241	-0.52757	S2E0O...0-..	2.20918	2.1148	0.16181	Omax.2.....	2.36141	0.00555	0.2832	n...s...1...	0.20567	-1.05538	-0.49937
O...2...3...	-0.77527	0.62546	-0.09644	S2E0O...1-..	-2.72368	-0.86438	-3.40428	Omax.3.....	0.50047	0.31377	0.45135	n...s...c...	2.03815	0.3696	0.67301
O...=...(...	-0.66784	0.08794	-0.71271	S2E0O...11-..	-0.44371	0.35183	-0.2497	Omax.4.....	-1.71576	-0.9249	-0.65231	o.....	0.58687	0.32538	2.25268
O...=.....	0.4887	-0.64317	-0.48616	S2E0O...2-..	-0.56127	2.21649	0.41584	Omax.5.....	-0.69226	-0.82128	0.27583	o...1.....	-1.41704	2.38201	1.77605
O...=...2...	-0.94348	-0.83997	0.16894	S2E0O...3-..	0.45322	-0.85291	-0.68519	VS2-C...10..	0.01544	0.46572	0.00187	o...1...c...	2.10296	2.63377	0.23094
O...=...C...	0.21476	0.09464	-0.94441	S2E0O...4-..	0.09143	-0.53168	-0.19205	VS2-C...11..	0.26752	0.36169	0.08777	o...c...(...	0.48243	2.03019	0.46509
O...C...(...	0.46772	-0.91689	-0.66502	S2E0O...5-..	0.08068	-0.74203	-0.88773	VS2-C...12..	0.49761	-0.8906	0.11889	o...c.....	0.28104	-0.74801	0.3194
O...C.....	0.29752	-0.04126	2.17112	S2E0O...6-..	0.38467	0.24995	0.18108	VS2-C...13..	-0.9202	0.31722	0.85729	s...(.....	-0.62742	0.6903	-0.35019
O...C...C...	0.37916	0.32285	2.10383	S2E0O...7-..	0.78233	-0.91691	-0.36489	VS2-C...14..	-0.17537	0.35764	-0.94554	s...(...1...	2.13886	0.46449	2.23479
O...C...O...	0.10613	-0.74936	-0.70609	S2E0O...8-..	-1.18507	1.87923	2.34376	VS2-C...15..	2.45706	0.13899	-0.77128	s...(...c...	-0.48347	-0.9438	0.27686
O...c...1...	-0.60562	-0.07472	-2.44684	S2E0O...9-..	0.14783	1.1461	0.28386	VS2-C...16..	0.03779	0.05445	0.16203	s.....	0.12998	0.40334	0.15193
O...c...2...	-0.34014	0.33535	0.32105	S2E0S...0-..	0.39132	0.35941	0.62512	VS2-C...17..	-0.93189	1.73812	2.59296	s...1...(...	-0.52863	0.25682	0.15824
P2E0C...0-..	2.31094	-0.87654	0.25368	S2E0S...1-..	0.17627	1.04204	0.07999	VS2-C...18..	0.43012	0.25189	0.37868	s...1.....	-0.85328	0.2643	0.13666
P2E0C...1-..	0.12128	2.05827	-0.91189	S2E0S...3-..	-0.92183	0.30118	-0.56522	VS2-C...2...	0.42671	0.13335	-0.82878	s...1...c...	0.23583	0.0517	-1.18805
P2E0C...2-..	0.06568	-0.64468	-0.90313	S2E0s...9-..	2.58245	0.32939	0.47675	VS2-C...3...	-0.76503	-0.73709	0.43779	s...2...(...	2.40492	-1.19031	1.38326
P2E0C...3-..	0.39576	0.27302	0.11615	S2E0s...5-..	1.91179	2.20513	0.068	VS2-C...4...	0.15362	0.17834	2.45033	s...2.....	0.28131	-0.41007	-1.11995
P2E0C...4-..	1.88206	-0.67798	2.10352	S2E0s...6-..	-1.9943	-1.55681	0.66099	VS2-C...5...	0.01704	0.42202	0.03643	s...c...(...	0.48126	0.3056	0.0661
P2E0F...1-..	4.30074	0.123	2.53355	S2E0s...8-..	-0.96886	-0.82281	0.52882	VS2-C...6...	-0.01596	0.20034	0.29228	s...c.....	2.09512	0.11647	0.39705

P2E0F...2-..	-0.28854	2.35994	-0.01594	S2E0s...9-..	0.19986	-0.77129	0.4668	VS2-C...7...	0.11826	0.49452	2.45151	s...c...1...	2.14398	0.39304	2.90501
P2E0Br..1-..	-1.3762	-0.8884	-0.71148	S3E0C...0-..	2.48867	-0.39634	-0.82467	VS2-C...8...	0.18354	0.08114	0.14307	s...c...2...	2.22247	0.30418	4.35731
P2E0Cl..1-..	1.25652	0.57676	2.86634	S3E0C...1-..	2.07158	2.13726	-0.07162	VS2-C...9...	0.23178	0.27463	0.18505	s...c...n...	0.13586	-0.12247	0.11923
P2E0Cl..2-..	-0.38335	-0.04562	2.27669	S3E0C...10-..	0.05045	-0.61465	0.30906	VS2-F...10..	2.1349	0.24968	0.49617	s...n...(...	2.21466	1.96561	0.37126
P2E0N...0-..	-0.29764	0.02209	-0.49053	S3E0C...11-..	0.16844	0.08131	-0.8326	VS2-F...4...	0.44264	0.88576	-0.58854	s...n.....	0.44911	-0.99348	-0.66839
P2E0N...1-..	-0.79136	0.48295	-0.67309	S3E0C...12-..	0.12831	-0.67711	0.12789	VS2-F...5...	1.17514	1.32373	2.13681	s...n...c...	-0.68496	0.38243	1.43116
P2E0N...2-..	-0.64336	-0.75617	1.12684	S3E0C...13-..	-0.99987	0.18875	-0.12138	VS2-F...6...	1.20755	0.97866	1.67693	s...n...n...	0.85497	0.41493	2.26696