

```

XTLGRF 200
DESCRP IS
REMARK Pt111_4x4x7_30.0_vac "top"-diffusion
FIXATOMS      1      32
CRYSTX      11.16485      11.16485      43.67409      90.00000      90.00000      60.00000
FORMAT ATOM      (a6,lx,i5,lx,a5,lx,a3,lx,a1,lx,a5,3f10.5,lx,a5,i3,i2,lx,f8.5)
HETATM      1 Pt      1.26492      9.26914      14.99394      Pt      1 0      0.00000
HETATM      2 Pt      1.26492      0.89550      14.99394      Pt      1 0      0.00000
HETATM      3 Pt      1.26492      3.68671      14.99394      Pt      1 0      0.00000
HETATM      4 Pt      1.26492      6.47793      14.99394      Pt      1 0      0.00000
HETATM      5 Pt      3.68218      10.66475      14.99394      Pt      1 0      0.00000
HETATM      6 Pt      3.68218      2.29111      14.99394      Pt      1 0      0.00000
HETATM      7 Pt      3.68218      5.08232      14.99394      Pt      1 0      0.00000
HETATM      8 Pt      3.68218      7.87353      14.99394      Pt      1 0      0.00000
HETATM      9 Pt      6.09944      12.06035      14.99394      Pt      1 0      0.00000
HETATM     10 Pt      6.09944      3.68671      14.99394      Pt      1 0      0.00000
HETATM     11 Pt      6.09944      6.47793      14.99394      Pt      1 0      0.00000
HETATM     12 Pt      6.09944      9.26914      14.99394      Pt      1 0      0.00000
HETATM     13 Pt      8.51670      13.45596      14.99394      Pt      1 0      0.00000
HETATM     14 Pt      8.51670      5.08232      14.99394      Pt      1 0      0.00000
HETATM     15 Pt      8.51670      7.87353      14.99394      Pt      1 0      0.00000
HETATM     16 Pt      8.51670      10.66474      14.99394      Pt      1 0      0.00000
HETATM     17 Pt      2.07067      10.66475      17.27296      Pt      1 0      0.00000
HETATM     18 Pt      2.07067      2.29111      17.27296      Pt      1 0      0.00000
HETATM     19 Pt      2.07067      5.08232      17.27296      Pt      1 0      0.00000
HETATM     20 Pt      2.07067      7.87353      17.27296      Pt      1 0      0.00000
HETATM     21 Pt      4.48793      12.06035      17.27296      Pt      1 0      0.00000
HETATM     22 Pt      4.48793      3.68671      17.27296      Pt      1 0      0.00000
HETATM     23 Pt      4.48793      6.47793      17.27296      Pt      1 0      0.00000
HETATM     24 Pt      4.48793      9.26914      17.27296      Pt      1 0      0.00000
HETATM     25 Pt      6.90519      13.45596      17.27296      Pt      1 0      0.00000
HETATM     26 Pt      6.90519      5.08232      17.27296      Pt      1 0      0.00000
HETATM     27 Pt      6.90519      7.87353      17.27296      Pt      1 0      0.00000
HETATM     28 Pt      6.90519      10.66474      17.27296      Pt      1 0      0.00000
HETATM     29 Pt      9.32246      14.85156      17.27296      Pt      1 0      0.00000
HETATM     30 Pt      9.32246      6.47793      17.27296      Pt      1 0      0.00000
HETATM     31 Pt      9.32246      9.26914      17.27296      Pt      1 0      0.00000
HETATM     32 Pt      9.32246      12.06035      17.27296      Pt      1 0      0.00000
HETATM     33 Pt      2.87620      12.05995      19.55145      Pt      1 0      0.00000
HETATM     34 Pt      2.87620      3.68710      19.55145      Pt      1 0      0.00000
HETATM     35 Pt      2.87668      6.47822      19.55122      Pt      1 0      0.00000
HETATM     36 Pt      2.87668      9.26884      19.55122      Pt      1 0      0.00000
HETATM     37 Pt      5.29414      13.45595      19.55145      Pt      1 0      0.00000
HETATM     38 Pt      5.29423      5.08327      19.55284      Pt      1 0      0.00000
HETATM     39 Pt      5.29424      7.87353      19.55392      Pt      1 0      0.00000
HETATM     40 Pt      5.29424      10.66379      19.55284      Pt      1 0      0.00000
HETATM     41 Pt      7.71107      14.85193      19.55122      Pt      1 0      0.00000
HETATM     42 Pt      7.71067      6.47841      19.55392      Pt      1 0      0.00000
HETATM     43 Pt      7.71067      9.26865      19.55392      Pt      1 0      0.00000
HETATM     44 Pt      7.71107      12.05998      19.55121      Pt      1 0      0.00000
HETATM     45 Pt      0.45879      10.66481      19.55122      Pt      1 0      0.00000
HETATM     46 Pt      0.45807      2.29110      19.55284      Pt      1 0      0.00000
HETATM     47 Pt      0.45879      5.08224      19.55122      Pt      1 0      0.00000
HETATM     48 Pt      0.45917      7.87352      19.55031      Pt      1 0      0.00000
HETATM     49 Pt      1.26489      9.26908      21.82821      Pt      1 0      0.00000
HETATM     50 Pt      1.26363      0.89540      21.83023      Pt      1 0      0.00000
HETATM     51 Pt      1.26363      3.68681      21.83023      Pt      1 0      0.00000
HETATM     52 Pt      1.26489      6.47798      21.82821      Pt      1 0      0.00000
HETATM     53 Pt      3.68274      10.66357      21.83023      Pt      1 0      0.00000
HETATM     54 Pt      3.68218      2.29110      21.82783      Pt      1 0      0.00000
HETATM     55 Pt      3.68274      5.08348      21.83023      Pt      1 0      0.00000
HETATM     56 Pt      3.68247      7.87353      21.83111      Pt      1 0      0.00000
HETATM     57 Pt      6.10017      12.05928      21.83023      Pt      1 0      0.00000

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HETATM	58	Pt	6.10017	3.68778	21.83023	Pt	1	0	0.00000
HETATM	59	Pt	6.10028	6.47938	21.83631	Pt	1	0	0.00000
HETATM	60	Pt	6.10028	9.26768	21.83631	Pt	1	0	0.00000
HETATM	61	Pt	8.51676	13.45595	21.82821	Pt	1	0	0.00000
HETATM	62	Pt	8.51656	5.08257	21.83111	Pt	1	0	0.00000
HETATM	63	Pt	8.51502	7.87353	21.83631	Pt	1	0	0.00000
HETATM	64	Pt	8.51656	10.66449	21.83111	Pt	1	0	0.00000
HETATM	65	Pt	2.07126	10.66576	24.10640	Pt	1	0	0.00000
HETATM	66	Pt	2.07194	2.29110	24.10578	Pt	1	0	0.00000
HETATM	67	Pt	2.07126	5.08130	24.10640	Pt	1	0	0.00000
HETATM	68	Pt	2.07012	7.87353	24.10630	Pt	1	0	0.00000
HETATM	69	Pt	4.48730	12.06144	24.10578	Pt	1	0	0.00000
HETATM	70	Pt	4.48730	3.68561	24.10578	Pt	1	0	0.00000
HETATM	71	Pt	4.48882	6.48053	24.11286	Pt	1	0	0.00000
HETATM	72	Pt	4.48882	9.26653	24.11286	Pt	1	0	0.00000
HETATM	73	Pt	6.90402	13.45595	24.10640	Pt	1	0	0.00000
HETATM	74	Pt	6.90701	5.08438	24.11286	Pt	1	0	0.00000
HETATM	75	Pt	6.90519	7.87353	24.12628	Pt	1	0	0.00000
HETATM	76	Pt	6.90701	10.66267	24.11286	Pt	1	0	0.00000
HETATM	77	Pt	9.32273	14.85108	24.10630	Pt	1	0	0.00000
HETATM	78	Pt	9.31976	6.47739	24.11286	Pt	1	0	0.00000
HETATM	79	Pt	9.31976	9.26967	24.11286	Pt	1	0	0.00000
HETATM	80	Pt	9.32273	12.06083	24.10630	Pt	1	0	0.00000
HETATM	81	Pt	2.87649	12.06045	26.39054	Pt	1	0	0.00000
HETATM	82	Pt	2.87649	3.68660	26.39054	Pt	1	0	0.00000
HETATM	83	Pt	2.87513	6.47490	26.38310	Pt	1	0	0.00000
HETATM	84	Pt	2.87513	9.27216	26.38310	Pt	1	0	0.00000
HETATM	85	Pt	5.29356	13.45595	26.39054	Pt	1	0	0.00000
HETATM	86	Pt	5.28774	5.07202	26.37641	Pt	1	0	0.00000
HETATM	87	Pt	5.29553	7.87353	26.41337	Pt	1	0	0.00000
HETATM	88	Pt	5.28774	10.67504	26.37641	Pt	1	0	0.00000
HETATM	89	Pt	7.70898	14.84893	26.38310	Pt	1	0	0.00000
HETATM	90	Pt	7.71002	6.47952	26.41337	Pt	1	0	0.00000
HETATM	91	Pt	7.71002	9.26754	26.41337	Pt	1	0	0.00000
HETATM	92	Pt	7.70898	12.06298	26.38310	Pt	1	0	0.00000
HETATM	93	Pt	0.46243	10.66513	26.38310	Pt	1	0	0.00000
HETATM	94	Pt	0.47106	2.29110	26.37641	Pt	1	0	0.00000
HETATM	95	Pt	0.46243	5.08192	26.38310	Pt	1	0	0.00000
HETATM	96	Pt	0.45917	7.87352	26.38396	Pt	1	0	0.00000
HETATM	97	Pt	1.26305	9.26590	28.66535	Pt	1	0	0.00000
HETATM	98	Pt	1.27189	0.88456	28.68535	Pt	1	0	0.00000
HETATM	99	Pt	1.27189	3.69765	28.68535	Pt	1	0	0.00000
HETATM	100	Pt	1.26305	6.48115	28.66535	Pt	1	0	0.00000
HETATM	101	Pt	3.66922	10.66531	28.68535	Pt	1	0	0.00000
HETATM	102	Pt	3.68218	2.29110	28.67188	Pt	1	0	0.00000
HETATM	103	Pt	3.66922	5.08175	28.68535	Pt	1	0	0.00000
HETATM	104	Pt	3.65327	7.87353	28.65048	Pt	1	0	0.00000
HETATM	105	Pt	6.10543	12.07185	28.68535	Pt	1	0	0.00000
HETATM	106	Pt	6.10543	3.67521	28.68535	Pt	1	0	0.00000
HETATM	107	Pt	6.10356	6.48505	28.74653	Pt	1	0	0.00000
HETATM	108	Pt	6.10355	9.26201	28.74653	Pt	1	0	0.00000
HETATM	109	Pt	8.52043	13.45595	28.66535	Pt	1	0	0.00000
HETATM	110	Pt	8.53116	5.05728	28.65048	Pt	1	0	0.00000
HETATM	111	Pt	8.50847	7.87353	28.74653	Pt	1	0	0.00000
HETATM	112	Pt	8.53116	10.68978	28.65048	Pt	1	0	0.00000
HETATM	113	O	6.90520	7.87353	29.86516	O	1	0	0.00000

UNIT ENERGY kcal
ENERGY -14466.434290
END

XTLGRF 200
DESCRP TS
REMARK Pt111_4x4x7_30.0_vac "top"-diffusion

FIXATOMS	1	32					
CRYSTX	11.16485	11.16485	43.67409	90.00000	90.00000	60.00000	
FORMAT	ATOM	(a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)					
HETATM	1	Pt	1.26550	9.27015	14.99394	Pt	1 0 0.00000
HETATM	2	Pt	1.26550	0.89651	14.99394	Pt	1 0 0.00000
HETATM	3	Pt	1.26550	3.68772	14.99394	Pt	1 0 0.00000
HETATM	4	Pt	1.26550	6.47894	14.99394	Pt	1 0 0.00000
HETATM	5	Pt	3.68276	10.66576	14.99394	Pt	1 0 0.00000
HETATM	6	Pt	3.68276	2.29212	14.99394	Pt	1 0 0.00000
HETATM	7	Pt	3.68276	5.08333	14.99394	Pt	1 0 0.00000
HETATM	8	Pt	3.68276	7.87454	14.99394	Pt	1 0 0.00000
HETATM	9	Pt	6.10002	12.06136	14.99394	Pt	1 0 0.00000
HETATM	10	Pt	6.10002	3.68772	14.99394	Pt	1 0 0.00000
HETATM	11	Pt	6.10002	6.47894	14.99394	Pt	1 0 0.00000
HETATM	12	Pt	6.10002	9.27015	14.99394	Pt	1 0 0.00000
HETATM	13	Pt	8.51728	13.45697	14.99394	Pt	1 0 0.00000
HETATM	14	Pt	8.51728	5.08333	14.99394	Pt	1 0 0.00000
HETATM	15	Pt	8.51728	7.87454	14.99394	Pt	1 0 0.00000
HETATM	16	Pt	8.51728	10.66575	14.99394	Pt	1 0 0.00000
HETATM	17	Pt	2.07125	10.66576	17.27296	Pt	1 0 0.00000
HETATM	18	Pt	2.07125	2.29212	17.27296	Pt	1 0 0.00000
HETATM	19	Pt	2.07125	5.08333	17.27296	Pt	1 0 0.00000
HETATM	20	Pt	2.07125	7.87454	17.27296	Pt	1 0 0.00000
HETATM	21	Pt	4.48851	12.06136	17.27296	Pt	1 0 0.00000
HETATM	22	Pt	4.48851	3.68772	17.27296	Pt	1 0 0.00000
HETATM	23	Pt	4.48851	6.47894	17.27296	Pt	1 0 0.00000
HETATM	24	Pt	4.48851	9.27015	17.27296	Pt	1 0 0.00000
HETATM	25	Pt	6.90577	13.45697	17.27296	Pt	1 0 0.00000
HETATM	26	Pt	6.90577	5.08333	17.27296	Pt	1 0 0.00000
HETATM	27	Pt	6.90577	7.87454	17.27296	Pt	1 0 0.00000
HETATM	28	Pt	6.90577	10.66575	17.27296	Pt	1 0 0.00000
HETATM	29	Pt	9.32304	14.85257	17.27296	Pt	1 0 0.00000
HETATM	30	Pt	9.32304	6.47894	17.27296	Pt	1 0 0.00000
HETATM	31	Pt	9.32304	9.27015	17.27296	Pt	1 0 0.00000
HETATM	32	Pt	9.32304	12.06136	17.27296	Pt	1 0 0.00000
HETATM	33	Pt	2.87708	12.06145	19.55050	Pt	1 0 0.00000
HETATM	34	Pt	2.87666	3.68786	19.55188	Pt	1 0 0.00000
HETATM	35	Pt	2.87686	6.47890	19.55177	Pt	1 0 0.00000
HETATM	36	Pt	2.87707	9.26994	19.55065	Pt	1 0 0.00000
HETATM	37	Pt	5.29457	13.45673	19.55188	Pt	1 0 0.00000
HETATM	38	Pt	5.29441	5.08355	19.55245	Pt	1 0 0.00000
HETATM	39	Pt	5.29458	7.87469	19.55248	Pt	1 0 0.00000
HETATM	40	Pt	5.29486	10.66552	19.55182	Pt	1 0 0.00000
HETATM	41	Pt	7.71161	14.85247	19.55177	Pt	1 0 0.00000
HETATM	42	Pt	7.71149	6.47927	19.55249	Pt	1 0 0.00000
HETATM	43	Pt	7.71162	9.27027	19.55293	Pt	1 0 0.00000
HETATM	44	Pt	7.71169	12.06093	19.55244	Pt	1 0 0.00000
HETATM	45	Pt	0.45956	10.66576	19.55065	Pt	1 0 0.00000
HETATM	46	Pt	0.45928	2.29251	19.55183	Pt	1 0 0.00000
HETATM	47	Pt	0.45935	5.08328	19.55245	Pt	1 0 0.00000
HETATM	48	Pt	0.45956	7.87419	19.55114	Pt	1 0 0.00000
HETATM	49	Pt	1.26533	9.26980	21.82801	Pt	1 0 0.00000
HETATM	50	Pt	1.26587	0.89705	21.82703	Pt	1 0 0.00000
HETATM	51	Pt	1.26445	3.68787	21.83170	Pt	1 0 0.00000
HETATM	52	Pt	1.26501	6.47870	21.83068	Pt	1 0 0.00000
HETATM	53	Pt	3.68305	10.66631	21.82702	Pt	1 0 0.00000
HETATM	54	Pt	3.68275	2.29206	21.82930	Pt	1 0 0.00000
HETATM	55	Pt	3.68237	5.08325	21.83066	Pt	1 0 0.00000
HETATM	56	Pt	3.68256	7.87449	21.82951	Pt	1 0 0.00000
HETATM	57	Pt	6.10069	12.06046	21.83170	Pt	1 0 0.00000
HETATM	58	Pt	6.10019	3.68730	21.83066	Pt	1 0 0.00000
HETATM	59	Pt	6.10035	6.47945	21.83165	Pt	1 0 0.00000
HETATM	60	Pt	6.10087	9.27047	21.83169	Pt	1 0 0.00000

HETATM	61	Pt	8.51739	13.45631	21.83068	Pt	1	0	0.00000
HETATM	62	Pt	8.51736	5.08310	21.82951	Pt	1	0	0.00000
HETATM	63	Pt	8.51717	7.87541	21.83170	Pt	1	0	0.00000
HETATM	64	Pt	8.51722	10.66560	21.83365	Pt	1	0	0.00000
HETATM	65	Pt	2.07210	10.66720	24.10146	Pt	1	0	0.00000
HETATM	66	Pt	2.07168	2.29266	24.10752	Pt	1	0	0.00000
HETATM	67	Pt	2.07012	5.08251	24.10994	Pt	1	0	0.00000
HETATM	68	Pt	2.07076	7.87451	24.10725	Pt	1	0	0.00000
HETATM	69	Pt	4.48877	12.06198	24.10751	Pt	1	0	0.00000
HETATM	70	Pt	4.48774	3.68639	24.10824	Pt	1	0	0.00000
HETATM	71	Pt	4.48805	6.47845	24.10769	Pt	1	0	0.00000
HETATM	72	Pt	4.48681	9.27454	24.10209	Pt	1	0	0.00000
HETATM	73	Pt	6.90559	13.45558	24.10993	Pt	1	0	0.00000
HETATM	74	Pt	6.90561	5.08269	24.10769	Pt	1	0	0.00000
HETATM	75	Pt	6.90674	7.87621	24.10959	Pt	1	0	0.00000
HETATM	76	Pt	6.90625	10.66471	24.11473	Pt	1	0	0.00000
HETATM	77	Pt	9.32325	14.85205	24.10724	Pt	1	0	0.00000
HETATM	78	Pt	9.32769	6.47963	24.10209	Pt	1	0	0.00000
HETATM	79	Pt	9.32191	9.27009	24.11474	Pt	1	0	0.00000
HETATM	80	Pt	9.32287	12.06108	24.11206	Pt	1	0	0.00000
HETATM	81	Pt	2.87743	12.06212	26.38420	Pt	1	0	0.00000
HETATM	82	Pt	2.87561	3.68642	26.38898	Pt	1	0	0.00000
HETATM	83	Pt	2.87476	6.47744	26.38340	Pt	1	0	0.00000
HETATM	84	Pt	2.87197	9.27705	26.37708	Pt	1	0	0.00000
HETATM	85	Pt	5.29382	13.45507	26.38898	Pt	1	0	0.00000
HETATM	86	Pt	5.28811	5.07265	26.38396	Pt	1	0	0.00000
HETATM	87	Pt	5.28243	7.89678	26.36640	Pt	1	0	0.00000
HETATM	88	Pt	5.29231	10.67242	26.38869	Pt	1	0	0.00000
HETATM	89	Pt	7.71136	14.84984	26.38340	Pt	1	0	0.00000
HETATM	90	Pt	7.73672	6.47981	26.36640	Pt	1	0	0.00000
HETATM	91	Pt	7.71072	9.26874	26.39849	Pt	1	0	0.00000
HETATM	92	Pt	7.71105	12.06116	26.39318	Pt	1	0	0.00000
HETATM	93	Pt	0.46821	10.66481	26.37707	Pt	1	0	0.00000
HETATM	94	Pt	0.46653	2.29377	26.38869	Pt	1	0	0.00000
HETATM	95	Pt	0.45980	5.08282	26.39318	Pt	1	0	0.00000
HETATM	96	Pt	0.45949	7.87406	26.38880	Pt	1	0	0.00000
HETATM	97	Pt	1.26613	9.27124	28.66541	Pt	1	0	0.00000
HETATM	98	Pt	1.26949	0.89453	28.66954	Pt	1	0	0.00000
HETATM	99	Pt	1.26792	3.68916	28.67951	Pt	1	0	0.00000
HETATM	100	Pt	1.26452	6.48226	28.67400	Pt	1	0	0.00000
HETATM	101	Pt	3.67906	10.66824	28.66954	Pt	1	0	0.00000
HETATM	102	Pt	3.68140	2.28976	28.66644	Pt	1	0	0.00000
HETATM	103	Pt	3.67558	5.08298	28.66912	Pt	1	0	0.00000
HETATM	104	Pt	3.67266	7.88512	28.63431	Pt	1	0	0.00000
HETATM	105	Pt	6.10008	12.06417	28.67951	Pt	1	0	0.00000
HETATM	106	Pt	6.10331	3.68133	28.66912	Pt	1	0	0.00000
HETATM	107	Pt	6.12150	6.51613	28.70762	Pt	1	0	0.00000
HETATM	108	Pt	6.09928	9.28927	28.67115	Pt	1	0	0.00000
HETATM	109	Pt	8.52062	13.45778	28.67400	Pt	1	0	0.00000
HETATM	110	Pt	8.53150	5.07986	28.63431	Pt	1	0	0.00000
HETATM	111	Pt	8.53425	7.88345	28.67115	Pt	1	0	0.00000
HETATM	112	Pt	8.52108	10.67228	28.67454	Pt	1	0	0.00000
HETATM	113	O	6.07456	6.43481	30.24819	O	1	0	0.00000

UNIT ENERGY kcal
ENERGY -14425.143357
END

XTLGRF 200
DESCRP FS
REMARK Pt111_4x4x7_30.0_vac "top"-diffusion
FIXATOMS 1 32
CRYSTX 11.16485 11.16485 43.67409 90.00000 90.00000 60.00000
FORMAT ATOM (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)

HETATM	1	Pt	1.26610	9.27118	14.99394	Pt	1	0	0.00000
HETATM	2	Pt	1.26610	0.89754	14.99394	Pt	1	0	0.00000
HETATM	3	Pt	1.26610	3.68875	14.99394	Pt	1	0	0.00000
HETATM	4	Pt	1.26610	6.47997	14.99394	Pt	1	0	0.00000
HETATM	5	Pt	3.68336	10.66679	14.99394	Pt	1	0	0.00000
HETATM	6	Pt	3.68336	2.29315	14.99394	Pt	1	0	0.00000
HETATM	7	Pt	3.68336	5.08436	14.99394	Pt	1	0	0.00000
HETATM	8	Pt	3.68336	7.87557	14.99394	Pt	1	0	0.00000
HETATM	9	Pt	6.10062	12.06239	14.99394	Pt	1	0	0.00000
HETATM	10	Pt	6.10062	3.68875	14.99394	Pt	1	0	0.00000
HETATM	11	Pt	6.10062	6.47997	14.99394	Pt	1	0	0.00000
HETATM	12	Pt	6.10062	9.27118	14.99394	Pt	1	0	0.00000
HETATM	13	Pt	8.51788	13.45800	14.99394	Pt	1	0	0.00000
HETATM	14	Pt	8.51788	5.08436	14.99394	Pt	1	0	0.00000
HETATM	15	Pt	8.51788	7.87557	14.99394	Pt	1	0	0.00000
HETATM	16	Pt	8.51788	10.66678	14.99394	Pt	1	0	0.00000
HETATM	17	Pt	2.07185	10.66679	17.27296	Pt	1	0	0.00000
HETATM	18	Pt	2.07185	2.29315	17.27296	Pt	1	0	0.00000
HETATM	19	Pt	2.07185	5.08436	17.27296	Pt	1	0	0.00000
HETATM	20	Pt	2.07185	7.87557	17.27296	Pt	1	0	0.00000
HETATM	21	Pt	4.48911	12.06239	17.27296	Pt	1	0	0.00000
HETATM	22	Pt	4.48911	3.68875	17.27296	Pt	1	0	0.00000
HETATM	23	Pt	4.48911	6.47997	17.27296	Pt	1	0	0.00000
HETATM	24	Pt	4.48911	9.27118	17.27296	Pt	1	0	0.00000
HETATM	25	Pt	6.90637	13.45800	17.27296	Pt	1	0	0.00000
HETATM	26	Pt	6.90637	5.08436	17.27296	Pt	1	0	0.00000
HETATM	27	Pt	6.90637	7.87557	17.27296	Pt	1	0	0.00000
HETATM	28	Pt	6.90637	10.66678	17.27296	Pt	1	0	0.00000
HETATM	29	Pt	9.32364	14.85360	17.27296	Pt	1	0	0.00000
HETATM	30	Pt	9.32364	6.47997	17.27296	Pt	1	0	0.00000
HETATM	31	Pt	9.32364	9.27118	17.27296	Pt	1	0	0.00000
HETATM	32	Pt	9.32364	12.06239	17.27296	Pt	1	0	0.00000
HETATM	33	Pt	2.87767	12.06251	19.55007	Pt	1	0	0.00000
HETATM	34	Pt	2.87706	3.68883	19.55232	Pt	1	0	0.00000
HETATM	35	Pt	2.87706	6.47989	19.55232	Pt	1	0	0.00000
HETATM	36	Pt	2.87767	9.27106	19.55007	Pt	1	0	0.00000
HETATM	37	Pt	5.29520	13.45757	19.55232	Pt	1	0	0.00000
HETATM	38	Pt	5.29486	5.08436	19.55250	Pt	1	0	0.00000
HETATM	39	Pt	5.29520	7.87600	19.55232	Pt	1	0	0.00000
HETATM	40	Pt	5.29570	10.66678	19.55189	Pt	1	0	0.00000
HETATM	41	Pt	7.71233	14.85310	19.55232	Pt	1	0	0.00000
HETATM	42	Pt	7.71233	6.48047	19.55232	Pt	1	0	0.00000
HETATM	43	Pt	7.71241	9.27166	19.55370	Pt	1	0	0.00000
HETATM	44	Pt	7.71241	12.06190	19.55370	Pt	1	0	0.00000
HETATM	45	Pt	0.46021	10.66679	19.55007	Pt	1	0	0.00000
HETATM	46	Pt	0.45993	2.29387	19.55189	Pt	1	0	0.00000
HETATM	47	Pt	0.45979	5.08436	19.55370	Pt	1	0	0.00000
HETATM	48	Pt	0.45993	7.87484	19.55189	Pt	1	0	0.00000
HETATM	49	Pt	1.26579	9.27065	21.82661	Pt	1	0	0.00000
HETATM	50	Pt	1.26579	0.89807	21.82661	Pt	1	0	0.00000
HETATM	51	Pt	1.26486	3.68927	21.83325	Pt	1	0	0.00000
HETATM	52	Pt	1.26486	6.47945	21.83325	Pt	1	0	0.00000
HETATM	53	Pt	3.68397	10.66678	21.82661	Pt	1	0	0.00000
HETATM	54	Pt	3.68287	2.29230	21.82900	Pt	1	0	0.00000
HETATM	55	Pt	3.68211	5.08436	21.83068	Pt	1	0	0.00000
HETATM	56	Pt	3.68287	7.87642	21.82900	Pt	1	0	0.00000
HETATM	57	Pt	6.10169	12.06157	21.83325	Pt	1	0	0.00000
HETATM	58	Pt	6.10124	3.68767	21.83068	Pt	1	0	0.00000
HETATM	59	Pt	6.10124	6.48105	21.83068	Pt	1	0	0.00000
HETATM	60	Pt	6.10169	9.27199	21.83325	Pt	1	0	0.00000
HETATM	61	Pt	8.51805	13.45666	21.83325	Pt	1	0	0.00000
HETATM	62	Pt	8.51885	5.08436	21.82900	Pt	1	0	0.00000
HETATM	63	Pt	8.51805	7.87691	21.83325	Pt	1	0	0.00000

HETATM	64	Pt	8.51788	10.66678	21.83693	Pt	1	0	0.00000
HETATM	65	Pt	2.07185	10.66678	24.09777	Pt	1	0	0.00000
HETATM	66	Pt	2.07019	2.29288	24.10706	Pt	1	0	0.00000
HETATM	67	Pt	2.07011	5.08436	24.11387	Pt	1	0	0.00000
HETATM	68	Pt	2.07019	7.87584	24.10706	Pt	1	0	0.00000
HETATM	69	Pt	4.48971	12.06082	24.10706	Pt	1	0	0.00000
HETATM	70	Pt	4.48847	3.68764	24.10566	Pt	1	0	0.00000
HETATM	71	Pt	4.48847	6.48108	24.10566	Pt	1	0	0.00000
HETATM	72	Pt	4.48971	9.27275	24.10706	Pt	1	0	0.00000
HETATM	73	Pt	6.90724	13.45649	24.11387	Pt	1	0	0.00000
HETATM	74	Pt	6.90766	5.08436	24.10566	Pt	1	0	0.00000
HETATM	75	Pt	6.90724	7.87708	24.11387	Pt	1	0	0.00000
HETATM	76	Pt	6.90760	10.66678	24.11939	Pt	1	0	0.00000
HETATM	77	Pt	9.32469	14.85230	24.10706	Pt	1	0	0.00000
HETATM	78	Pt	9.32469	6.48127	24.10706	Pt	1	0	0.00000
HETATM	79	Pt	9.32302	9.27224	24.11939	Pt	1	0	0.00000
HETATM	80	Pt	9.32302	12.06132	24.11939	Pt	1	0	0.00000
HETATM	81	Pt	2.87473	12.05740	26.37463	Pt	1	0	0.00000
HETATM	82	Pt	2.88020	3.68373	26.38642	Pt	1	0	0.00000
HETATM	83	Pt	2.88020	6.48499	26.38642	Pt	1	0	0.00000
HETATM	84	Pt	2.87473	9.27616	26.37463	Pt	1	0	0.00000
HETATM	85	Pt	5.28922	13.45773	26.38642	Pt	1	0	0.00000
HETATM	86	Pt	5.29487	5.08436	26.38057	Pt	1	0	0.00000
HETATM	87	Pt	5.28922	7.87584	26.38642	Pt	1	0	0.00000
HETATM	88	Pt	5.29505	10.66678	26.39395	Pt	1	0	0.00000
HETATM	89	Pt	7.71518	14.85836	26.38642	Pt	1	0	0.00000
HETATM	90	Pt	7.71518	6.47520	26.38642	Pt	1	0	0.00000
HETATM	91	Pt	7.71093	9.26910	26.40653	Pt	1	0	0.00000
HETATM	92	Pt	7.71093	12.06447	26.40653	Pt	1	0	0.00000
HETATM	93	Pt	0.46611	10.66679	26.37463	Pt	1	0	0.00000
HETATM	94	Pt	0.46026	2.29331	26.39395	Pt	1	0	0.00000
HETATM	95	Pt	0.46275	5.08436	26.40653	Pt	1	0	0.00000
HETATM	96	Pt	0.46026	7.87541	26.39395	Pt	1	0	0.00000
HETATM	97	Pt	1.26930	9.27672	28.66373	Pt	1	0	0.00000
HETATM	98	Pt	1.26930	0.89200	28.66373	Pt	1	0	0.00000
HETATM	99	Pt	1.25674	3.67416	28.69497	Pt	1	0	0.00000
HETATM	100	Pt	1.25674	6.49455	28.69497	Pt	1	0	0.00000
HETATM	101	Pt	3.67696	10.66678	28.66373	Pt	1	0	0.00000
HETATM	102	Pt	3.66995	2.26992	28.64375	Pt	1	0	0.00000
HETATM	103	Pt	3.66736	5.08436	28.73828	Pt	1	0	0.00000
HETATM	104	Pt	3.66995	7.89880	28.64375	Pt	1	0	0.00000
HETATM	105	Pt	6.09266	12.04700	28.69497	Pt	1	0	0.00000
HETATM	106	Pt	6.10862	3.67490	28.73828	Pt	1	0	0.00000
HETATM	107	Pt	6.10862	6.49382	28.73828	Pt	1	0	0.00000
HETATM	108	Pt	6.09266	9.28657	28.69497	Pt	1	0	0.00000
HETATM	109	Pt	8.53519	13.45719	28.69497	Pt	1	0	0.00000
HETATM	110	Pt	8.54470	5.08436	28.64375	Pt	1	0	0.00000
HETATM	111	Pt	8.53519	7.87638	28.69497	Pt	1	0	0.00000
HETATM	112	Pt	8.51788	10.66678	28.68932	Pt	1	0	0.00000
HETATM	113	O	5.29487	5.08436	29.84788	O	1	0	0.00000
UNIT ENERGY kcal									
ENERGY -14462.712538									
END									