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XTLGRF 200
DESCRP A0080
REMARK Pt111_clean_1x1x14_30.0_vac
FIXATOMS      7      8
CRYSTX      2.79121      2.79121      59.62720      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      -0.00000      0.00000      -0.00117      Pt      1 0      0.00000
HETATM      2 Pt      0.80575      1.39561      2.28018      Pt      1 0      0.00000
HETATM      3 Pt      1.61151      2.79121      4.55805      Pt      1 0      0.00000
HETATM      4 Pt      0.00000      0.00000      6.83705      Pt      1 0      0.00000
HETATM      5 Pt      0.80575      1.39561      9.11606      Pt      1 0      0.00000
HETATM      6 Pt      1.61151      2.79121      11.39508      Pt      1 0      0.00000
HETATM      7 Pt      0.00000      0.00000      13.67409      Pt      1 0      0.00000
HETATM      8 Pt      0.80575      1.39561      15.95311      Pt      1 0      0.00000
HETATM      9 Pt      1.61151      2.79121      18.23212      Pt      1 0      0.00000
HETATM     10 Pt      0.00000      0.00000      20.51114      Pt      1 0      0.00000
HETATM     11 Pt      0.80575      1.39561      22.79015      Pt      1 0      0.00000
HETATM     12 Pt      1.61151      2.79121      25.06915      Pt      1 0      0.00000
HETATM     13 Pt      0.00000      0.00000      27.34702      Pt      1 0      0.00000
HETATM     14 Pt      0.80575      1.39561      29.62837      Pt      1 0      0.00000
UNIT ENERGY      kcal
ENERGY      -1830.353178
END

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XTLGRF 200
DESCRP A0050
REMARK Pt111_0.11ML_3x3x14_30.0_vac
FIXATOMS     55     72
CRYSTX      8.37364      8.37364      59.62720      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      -0.00942      -0.01631      0.01711      Pt      1 0      0.00000
HETATM      2 Pt      0.01171      2.79121      -0.08297      Pt      1 0      0.00000
HETATM      3 Pt      -0.00942      5.59873      0.01711      Pt      1 0      0.00000
HETATM      4 Pt      2.41140      1.40575      -0.08297      Pt      1 0      0.00000
HETATM      5 Pt      2.41140      4.17667      -0.08297      Pt      1 0      0.00000
HETATM      6 Pt      2.40638      6.97803      -0.03628      Pt      1 0      0.00000
HETATM      7 Pt      4.85335      2.79121      0.01711      Pt      1 0      0.00000
HETATM      8 Pt      4.83996      5.57300      -0.03628      Pt      1 0      0.00000
HETATM      9 Pt      4.83996      8.38306      -0.03628      Pt      1 0      0.00000
HETATM     10 Pt      0.80788      1.39929      2.25508      Pt      1 0      0.00000
HETATM     11 Pt      0.80788      4.18313      2.25508      Pt      1 0      0.00000
HETATM     12 Pt      0.80898      6.97803      2.28406      Pt      1 0      0.00000
HETATM     13 Pt      3.21876      2.79121      2.25508      Pt      1 0      0.00000
HETATM     14 Pt      3.22730      5.58985      2.28660      Pt      1 0      0.00000
HETATM     15 Pt      3.22730      8.36621      2.28660      Pt      1 0      0.00000
HETATM     16 Pt      5.63866      4.18961      2.28406      Pt      1 0      0.00000
HETATM     17 Pt      5.63170      6.97803      2.28660      Pt      1 0      0.00000
HETATM     18 Pt      5.63866      9.76645      2.28406      Pt      1 0      0.00000
HETATM     19 Pt      1.61151      2.79121      4.54447      Pt      1 0      0.00000
HETATM     20 Pt      1.60984      5.58042      4.55459      Pt      1 0      0.00000
HETATM     21 Pt      1.60984      8.37564      4.55459      Pt      1 0      0.00000
HETATM     22 Pt      4.02786      4.18438      4.55459      Pt      1 0      0.00000
HETATM     23 Pt      4.02877      6.97803      4.56453      Pt      1 0      0.00000
HETATM     24 Pt      4.02786      9.77168      4.55459      Pt      1 0      0.00000
HETATM     25 Pt      6.44859      5.58199      4.55459      Pt      1 0      0.00000
HETATM     26 Pt      6.44859      8.37408      4.55459      Pt      1 0      0.00000
HETATM     27 Pt      6.44603      11.16485      4.56012      Pt      1 0      0.00000
HETATM     28 Pt      0.00007      0.00012      6.83691      Pt      1 0      0.00000
HETATM     29 Pt      0.00094      2.79121      6.83217      Pt      1 0      0.00000
HETATM     30 Pt      0.00007      5.58230      6.83691      Pt      1 0      0.00000
HETATM     31 Pt      2.41679      1.39642      6.83217      Pt      1 0      0.00000
HETATM     32 Pt      2.41679      4.18600      6.83217      Pt      1 0      0.00000
HETATM     33 Pt      2.41598      6.97803      6.83584      Pt      1 0      0.00000

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HETATM	34	Pt	4.83438	2.79121	6.83691	Pt	1	0	0.00000
HETATM	35	Pt	4.83516	5.58132	6.83584	Pt	1	0	0.00000
HETATM	36	Pt	4.83516	8.37474	6.83584	Pt	1	0	0.00000
HETATM	37	Pt	0.80601	1.39605	9.11386	Pt	1	0	0.00000
HETATM	38	Pt	0.80601	4.18637	9.11386	Pt	1	0	0.00000
HETATM	39	Pt	0.80568	6.97803	9.11608	Pt	1	0	0.00000
HETATM	40	Pt	3.22250	2.79121	9.11386	Pt	1	0	0.00000
HETATM	41	Pt	3.22274	5.58196	9.11348	Pt	1	0	0.00000
HETATM	42	Pt	3.22274	8.37410	9.11348	Pt	1	0	0.00000
HETATM	43	Pt	5.64031	4.18676	9.11608	Pt	1	0	0.00000
HETATM	44	Pt	5.64081	6.97803	9.11348	Pt	1	0	0.00000
HETATM	45	Pt	5.64031	9.76931	9.11608	Pt	1	0	0.00000
HETATM	46	Pt	1.61151	2.79121	11.39423	Pt	1	0	0.00000
HETATM	47	Pt	1.61165	5.58220	11.39414	Pt	1	0	0.00000
HETATM	48	Pt	1.61165	8.37386	11.39414	Pt	1	0	0.00000
HETATM	49	Pt	4.02850	4.18683	11.39414	Pt	1	0	0.00000
HETATM	50	Pt	4.02877	6.97803	11.39303	Pt	1	0	0.00000
HETATM	51	Pt	4.02850	9.76923	11.39414	Pt	1	0	0.00000
HETATM	52	Pt	6.44615	5.58266	11.39414	Pt	1	0	0.00000
HETATM	53	Pt	6.44615	8.37340	11.39414	Pt	1	0	0.00000
HETATM	54	Pt	6.44603	11.16485	11.39519	Pt	1	0	0.00000
HETATM	55	Pt	0.00000	0.00000	13.67409	Pt	1	0	0.00000
HETATM	56	Pt	0.00000	2.79121	13.67409	Pt	1	0	0.00000
HETATM	57	Pt	0.00000	5.58242	13.67409	Pt	1	0	0.00000
HETATM	58	Pt	2.41726	1.39561	13.67409	Pt	1	0	0.00000
HETATM	59	Pt	2.41726	4.18682	13.67409	Pt	1	0	0.00000
HETATM	60	Pt	2.41726	6.97803	13.67409	Pt	1	0	0.00000
HETATM	61	Pt	4.83452	2.79121	13.67409	Pt	1	0	0.00000
HETATM	62	Pt	4.83452	5.58242	13.67409	Pt	1	0	0.00000
HETATM	63	Pt	4.83452	8.37364	13.67409	Pt	1	0	0.00000
HETATM	64	Pt	0.80575	1.39561	15.95311	Pt	1	0	0.00000
HETATM	65	Pt	0.80575	4.18682	15.95311	Pt	1	0	0.00000
HETATM	66	Pt	0.80575	6.97803	15.95311	Pt	1	0	0.00000
HETATM	67	Pt	3.22301	2.79121	15.95311	Pt	1	0	0.00000
HETATM	68	Pt	3.22301	5.58242	15.95311	Pt	1	0	0.00000
HETATM	69	Pt	3.22301	8.37364	15.95311	Pt	1	0	0.00000
HETATM	70	Pt	5.64027	4.18682	15.95311	Pt	1	0	0.00000
HETATM	71	Pt	5.64027	6.97803	15.95311	Pt	1	0	0.00000
HETATM	72	Pt	5.64027	9.76924	15.95311	Pt	1	0	0.00000
HETATM	73	Pt	1.61150	2.79121	18.23297	Pt	1	0	0.00000
HETATM	74	Pt	1.61136	5.58220	18.23306	Pt	1	0	0.00000
HETATM	75	Pt	1.61136	8.37386	18.23306	Pt	1	0	0.00000
HETATM	76	Pt	4.02864	4.18658	18.23306	Pt	1	0	0.00000
HETATM	77	Pt	4.02876	6.97803	18.23201	Pt	1	0	0.00000
HETATM	78	Pt	4.02864	9.76948	18.23306	Pt	1	0	0.00000
HETATM	79	Pt	6.44630	5.58241	18.23306	Pt	1	0	0.00000
HETATM	80	Pt	6.44630	8.37365	18.23306	Pt	1	0	0.00000
HETATM	81	Pt	6.44603	11.16485	18.23417	Pt	1	0	0.00000
HETATM	82	Pt	0.00027	0.00046	20.51372	Pt	1	0	0.00000
HETATM	83	Pt	0.00051	2.79121	20.51334	Pt	1	0	0.00000
HETATM	84	Pt	0.00027	5.58196	20.51372	Pt	1	0	0.00000
HETATM	85	Pt	2.41700	1.39605	20.51334	Pt	1	0	0.00000
HETATM	86	Pt	2.41700	4.18637	20.51334	Pt	1	0	0.00000
HETATM	87	Pt	2.41733	6.97803	20.51112	Pt	1	0	0.00000
HETATM	88	Pt	4.83398	2.79121	20.51372	Pt	1	0	0.00000
HETATM	89	Pt	4.83449	5.58249	20.51112	Pt	1	0	0.00000
HETATM	90	Pt	4.83449	8.37358	20.51112	Pt	1	0	0.00000
HETATM	91	Pt	0.80622	1.39642	22.79503	Pt	1	0	0.00000
HETATM	92	Pt	0.80622	4.18600	22.79503	Pt	1	0	0.00000
HETATM	93	Pt	0.80703	6.97803	22.79136	Pt	1	0	0.00000
HETATM	94	Pt	3.22207	2.79121	22.79503	Pt	1	0	0.00000
HETATM	95	Pt	3.22294	5.58230	22.79029	Pt	1	0	0.00000
HETATM	96	Pt	3.22294	8.37376	22.79029	Pt	1	0	0.00000

HETATM	97	Pt	5.63964	4.18792	22.79136	Pt	1	0	0.00000
HETATM	98	Pt	5.64042	6.97803	22.79029	Pt	1	0	0.00000
HETATM	99	Pt	5.63964	9.76814	22.79136	Pt	1	0	0.00000
HETATM	100	Pt	1.61151	2.79121	25.08273	Pt	1	0	0.00000
HETATM	101	Pt	1.61317	5.58042	25.07261	Pt	1	0	0.00000
HETATM	102	Pt	1.61317	8.37564	25.07261	Pt	1	0	0.00000
HETATM	103	Pt	4.02620	4.18726	25.07261	Pt	1	0	0.00000
HETATM	104	Pt	4.02877	6.97803	25.06708	Pt	1	0	0.00000
HETATM	105	Pt	4.02620	9.76881	25.07261	Pt	1	0	0.00000
HETATM	106	Pt	6.44693	5.58486	25.07261	Pt	1	0	0.00000
HETATM	107	Pt	6.44693	8.37120	25.07261	Pt	1	0	0.00000
HETATM	108	Pt	6.44603	11.16485	25.06267	Pt	1	0	0.00000
HETATM	109	Pt	-0.00429	-0.00743	27.34060	Pt	1	0	0.00000
HETATM	110	Pt	0.00425	2.79121	27.37212	Pt	1	0	0.00000
HETATM	111	Pt	-0.00429	5.58985	27.34060	Pt	1	0	0.00000
HETATM	112	Pt	2.41513	1.39929	27.37212	Pt	1	0	0.00000
HETATM	113	Pt	2.41513	4.18313	27.37212	Pt	1	0	0.00000
HETATM	114	Pt	2.41403	6.97803	27.34314	Pt	1	0	0.00000
HETATM	115	Pt	4.84310	2.79121	27.34060	Pt	1	0	0.00000
HETATM	116	Pt	4.83613	5.57963	27.34314	Pt	1	0	0.00000
HETATM	117	Pt	4.83613	8.37643	27.34314	Pt	1	0	0.00000
HETATM	118	Pt	0.81161	1.40575	29.71017	Pt	1	0	0.00000
HETATM	119	Pt	0.81161	4.17667	29.71017	Pt	1	0	0.00000
HETATM	120	Pt	0.81663	6.97803	29.66348	Pt	1	0	0.00000
HETATM	121	Pt	3.21130	2.79121	29.71017	Pt	1	0	0.00000
HETATM	122	Pt	3.23243	5.59873	29.61009	Pt	1	0	0.00000
HETATM	123	Pt	3.23243	8.35733	29.61009	Pt	1	0	0.00000
HETATM	124	Pt	5.63483	4.19624	29.66348	Pt	1	0	0.00000
HETATM	125	Pt	5.62145	6.97803	29.61009	Pt	1	0	0.00000
HETATM	126	Pt	5.63483	9.75982	29.66348	Pt	1	0	0.00000
HETATM	127	O	1.61151	2.79121	30.82998	O	1	0	0.00000
HETATM	128	O	1.61151	2.79121	-1.20278	O	1	0	0.00000

UNIT ENERGY kcal
ENERGY -16648.546290
END

XTLGRF 200
DESCRP A0014
REMARK Pt111_0.25ML_2x2x14_30.0_vac
FIXATOMS 25 32
CRYSTX 5.58242 5.58242 59.62720 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	0.00000	0.00000	0.04665	Pt	1	0	0.00000
HETATM	2	Pt	0.02539	2.79121	-0.12271	Pt	1	0	0.00000
HETATM	3	Pt	2.40456	1.41760	-0.12271	Pt	1	0	0.00000
HETATM	4	Pt	2.40456	4.16483	-0.12271	Pt	1	0	0.00000
HETATM	5	Pt	0.81031	1.40350	2.25522	Pt	1	0	0.00000
HETATM	6	Pt	0.81031	4.17893	2.25522	Pt	1	0	0.00000
HETATM	7	Pt	3.21390	2.79121	2.25522	Pt	1	0	0.00000
HETATM	8	Pt	3.22301	5.58242	2.33175	Pt	1	0	0.00000
HETATM	9	Pt	1.61151	2.79121	4.54638	Pt	1	0	0.00000
HETATM	10	Pt	1.60536	5.58242	4.55888	Pt	1	0	0.00000
HETATM	11	Pt	4.03184	4.18149	4.55888	Pt	1	0	0.00000
HETATM	12	Pt	4.03184	6.98335	4.55888	Pt	1	0	0.00000
HETATM	13	Pt	0.00000	0.00000	6.83995	Pt	1	0	0.00000
HETATM	14	Pt	0.00085	2.79121	6.83408	Pt	1	0	0.00000
HETATM	15	Pt	2.41683	1.39635	6.83407	Pt	1	0	0.00000
HETATM	16	Pt	2.41683	4.18608	6.83407	Pt	1	0	0.00000
HETATM	17	Pt	0.80597	1.39598	9.11560	Pt	1	0	0.00000
HETATM	18	Pt	0.80597	4.18644	9.11560	Pt	1	0	0.00000
HETATM	19	Pt	3.22258	2.79121	9.11560	Pt	1	0	0.00000
HETATM	20	Pt	3.22301	5.58242	9.11379	Pt	1	0	0.00000
HETATM	21	Pt	1.61151	2.79121	11.39494	Pt	1	0	0.00000

HETATM	22	Pt	1.61163	5.58242	11.39431	Pt	1	0	0.00000
HETATM	23	Pt	4.02870	4.18693	11.39431	Pt	1	0	0.00000
HETATM	24	Pt	4.02870	6.97792	11.39431	Pt	1	0	0.00000
HETATM	25	Pt	0.00000	0.00000	13.67409	Pt	1	0	0.00000
HETATM	26	Pt	0.00000	2.79121	13.67409	Pt	1	0	0.00000
HETATM	27	Pt	2.41726	1.39561	13.67409	Pt	1	0	0.00000
HETATM	28	Pt	2.41726	4.18682	13.67409	Pt	1	0	0.00000
HETATM	29	Pt	0.80575	1.39561	15.95311	Pt	1	0	0.00000
HETATM	30	Pt	0.80575	4.18682	15.95311	Pt	1	0	0.00000
HETATM	31	Pt	3.22301	2.79121	15.95311	Pt	1	0	0.00000
HETATM	32	Pt	3.22301	5.58242	15.95311	Pt	1	0	0.00000
HETATM	33	Pt	1.61151	2.79121	18.23226	Pt	1	0	0.00000
HETATM	34	Pt	1.61138	5.58242	18.23289	Pt	1	0	0.00000
HETATM	35	Pt	4.02883	4.18671	18.23289	Pt	1	0	0.00000
HETATM	36	Pt	4.02883	6.97814	18.23289	Pt	1	0	0.00000
HETATM	37	Pt	0.00000	0.00000	20.51341	Pt	1	0	0.00000
HETATM	38	Pt	0.00043	2.79121	20.51160	Pt	1	0	0.00000
HETATM	39	Pt	2.41704	1.39598	20.51160	Pt	1	0	0.00000
HETATM	40	Pt	2.41704	4.18644	20.51160	Pt	1	0	0.00000
HETATM	41	Pt	0.80618	1.39635	22.79312	Pt	1	0	0.00000
HETATM	42	Pt	0.80618	4.18608	22.79312	Pt	1	0	0.00000
HETATM	43	Pt	3.22216	2.79121	22.79312	Pt	1	0	0.00000
HETATM	44	Pt	3.22301	5.58242	22.78725	Pt	1	0	0.00000
HETATM	45	Pt	1.61151	2.79121	25.08082	Pt	1	0	0.00000
HETATM	46	Pt	1.61765	5.58242	25.06832	Pt	1	0	0.00000
HETATM	47	Pt	4.02569	4.19214	25.06832	Pt	1	0	0.00000
HETATM	48	Pt	4.02569	6.97270	25.06832	Pt	1	0	0.00000
HETATM	49	Pt	0.00000	0.00000	27.29545	Pt	1	0	0.00000
HETATM	50	Pt	0.00911	2.79121	27.37198	Pt	1	0	0.00000
HETATM	51	Pt	2.41270	1.40350	27.37198	Pt	1	0	0.00000
HETATM	52	Pt	2.41270	4.17893	27.37198	Pt	1	0	0.00000
HETATM	53	Pt	0.81845	1.41760	29.74991	Pt	1	0	0.00000
HETATM	54	Pt	0.81845	4.16483	29.74991	Pt	1	0	0.00000
HETATM	55	Pt	3.19762	2.79121	29.74991	Pt	1	0	0.00000
HETATM	56	Pt	3.22301	5.58242	29.58055	Pt	1	0	0.00000
HETATM	57	O	1.61151	2.79121	30.86935	O	1	0	0.00000
HETATM	58	O	1.61151	2.79121	-1.24215	O	1	0	0.00000

UNIT ENERGY kcal
ENERGY -7502.498169
END

XTLGRF 200
DESCRP A0106
REMARK Pt111_0.33ML_3x3x14_30.0_vac
FIXATOMS 55 72
CRYSTX 8.37364 8.37364 59.62720 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	-0.00924	-0.01601	-0.09408	Pt	1	0	0.00000
HETATM	2	Pt	0.01848	2.79121	-0.09408	Pt	1	0	0.00000
HETATM	3	Pt	-0.00924	5.59843	-0.09408	Pt	1	0	0.00000
HETATM	4	Pt	2.40802	1.41161	-0.09408	Pt	1	0	0.00000
HETATM	5	Pt	2.40802	4.17081	-0.09408	Pt	1	0	0.00000
HETATM	6	Pt	2.43574	6.97803	-0.09408	Pt	1	0	0.00000
HETATM	7	Pt	4.85300	2.79121	-0.09408	Pt	1	0	0.00000
HETATM	8	Pt	4.82528	5.59843	-0.09408	Pt	1	0	0.00000
HETATM	9	Pt	4.82528	8.35763	-0.09408	Pt	1	0	0.00000
HETATM	10	Pt	0.81068	1.40414	2.26861	Pt	1	0	0.00000
HETATM	11	Pt	0.81068	4.17828	2.26861	Pt	1	0	0.00000
HETATM	12	Pt	0.79590	6.97803	2.26861	Pt	1	0	0.00000
HETATM	13	Pt	3.21316	2.79121	2.26861	Pt	1	0	0.00000
HETATM	14	Pt	3.22794	5.59096	2.26861	Pt	1	0	0.00000
HETATM	15	Pt	3.22794	8.36510	2.26861	Pt	1	0	0.00000
HETATM	16	Pt	5.64520	4.17828	2.26861	Pt	1	0	0.00000

HETATM	17	Pt	5.63042	6.97803	2.26861	Pt	1	0	0.00000
HETATM	18	Pt	5.64520	9.77778	2.26861	Pt	1	0	0.00000
HETATM	19	Pt	1.61151	2.79121	4.55324	Pt	1	0	0.00000
HETATM	20	Pt	1.61151	5.58242	4.54701	Pt	1	0	0.00000
HETATM	21	Pt	1.61151	8.37364	4.54701	Pt	1	0	0.00000
HETATM	22	Pt	4.02877	4.18682	4.54701	Pt	1	0	0.00000
HETATM	23	Pt	4.02877	6.97803	4.55324	Pt	1	0	0.00000
HETATM	24	Pt	4.02877	9.76924	4.54701	Pt	1	0	0.00000
HETATM	25	Pt	6.44603	5.58242	4.54701	Pt	1	0	0.00000
HETATM	26	Pt	6.44603	8.37364	4.54701	Pt	1	0	0.00000
HETATM	27	Pt	6.44603	11.16485	4.55324	Pt	1	0	0.00000
HETATM	28	Pt	0.00030	0.00052	6.83003	Pt	1	0	0.00000
HETATM	29	Pt	-0.00061	2.79121	6.83003	Pt	1	0	0.00000
HETATM	30	Pt	0.00030	5.58190	6.83003	Pt	1	0	0.00000
HETATM	31	Pt	2.41756	1.39508	6.83003	Pt	1	0	0.00000
HETATM	32	Pt	2.41756	4.18734	6.83003	Pt	1	0	0.00000
HETATM	33	Pt	2.41666	6.97803	6.83003	Pt	1	0	0.00000
HETATM	34	Pt	4.83392	2.79121	6.83003	Pt	1	0	0.00000
HETATM	35	Pt	4.83482	5.58190	6.83003	Pt	1	0	0.00000
HETATM	36	Pt	4.83482	8.37416	6.83003	Pt	1	0	0.00000
HETATM	37	Pt	0.80578	1.39565	9.11104	Pt	1	0	0.00000
HETATM	38	Pt	0.80578	4.18678	9.11104	Pt	1	0	0.00000
HETATM	39	Pt	0.80570	6.97803	9.11104	Pt	1	0	0.00000
HETATM	40	Pt	3.22297	2.79121	9.11104	Pt	1	0	0.00000
HETATM	41	Pt	3.22304	5.58247	9.11104	Pt	1	0	0.00000
HETATM	42	Pt	3.22304	8.37360	9.11104	Pt	1	0	0.00000
HETATM	43	Pt	5.64030	4.18678	9.11104	Pt	1	0	0.00000
HETATM	44	Pt	5.64023	6.97803	9.11104	Pt	1	0	0.00000
HETATM	45	Pt	5.64030	9.76929	9.11104	Pt	1	0	0.00000
HETATM	46	Pt	1.61151	2.79121	11.39217	Pt	1	0	0.00000
HETATM	47	Pt	1.61151	5.58242	11.39215	Pt	1	0	0.00000
HETATM	48	Pt	1.61151	8.37364	11.39216	Pt	1	0	0.00000
HETATM	49	Pt	4.02877	4.18682	11.39215	Pt	1	0	0.00000
HETATM	50	Pt	4.02877	6.97803	11.39217	Pt	1	0	0.00000
HETATM	51	Pt	4.02877	9.76924	11.39215	Pt	1	0	0.00000
HETATM	52	Pt	6.44603	5.58242	11.39215	Pt	1	0	0.00000
HETATM	53	Pt	6.44603	8.37364	11.39215	Pt	1	0	0.00000
HETATM	54	Pt	6.44603	11.16485	11.39217	Pt	1	0	0.00000
HETATM	55	Pt	0.00000	0.00000	13.67409	Pt	1	0	0.00000
HETATM	56	Pt	0.00000	2.79121	13.67409	Pt	1	0	0.00000
HETATM	57	Pt	0.00000	5.58242	13.67409	Pt	1	0	0.00000
HETATM	58	Pt	2.41726	1.39561	13.67409	Pt	1	0	0.00000
HETATM	59	Pt	2.41726	4.18682	13.67409	Pt	1	0	0.00000
HETATM	60	Pt	2.41726	6.97803	13.67409	Pt	1	0	0.00000
HETATM	61	Pt	4.83452	2.79121	13.67409	Pt	1	0	0.00000
HETATM	62	Pt	4.83452	5.58242	13.67409	Pt	1	0	0.00000
HETATM	63	Pt	4.83452	8.37364	13.67409	Pt	1	0	0.00000
HETATM	64	Pt	0.80575	1.39561	15.95311	Pt	1	0	0.00000
HETATM	65	Pt	0.80575	4.18682	15.95311	Pt	1	0	0.00000
HETATM	66	Pt	0.80575	6.97803	15.95311	Pt	1	0	0.00000
HETATM	67	Pt	3.22301	2.79121	15.95311	Pt	1	0	0.00000
HETATM	68	Pt	3.22301	5.58242	15.95311	Pt	1	0	0.00000
HETATM	69	Pt	3.22301	8.37364	15.95311	Pt	1	0	0.00000
HETATM	70	Pt	5.64027	4.18682	15.95311	Pt	1	0	0.00000
HETATM	71	Pt	5.64027	6.97803	15.95311	Pt	1	0	0.00000
HETATM	72	Pt	5.64027	9.76924	15.95311	Pt	1	0	0.00000
HETATM	73	Pt	1.61150	2.79121	18.23503	Pt	1	0	0.00000
HETATM	74	Pt	1.61150	5.58242	18.23505	Pt	1	0	0.00000
HETATM	75	Pt	1.61150	8.37364	18.23505	Pt	1	0	0.00000
HETATM	76	Pt	4.02877	4.18682	18.23505	Pt	1	0	0.00000
HETATM	77	Pt	4.02876	6.97803	18.23503	Pt	1	0	0.00000
HETATM	78	Pt	4.02877	9.76924	18.23505	Pt	1	0	0.00000
HETATM	79	Pt	6.44603	5.58242	18.23505	Pt	1	0	0.00000

HETATM	80	Pt	6.44603	8.37364	18.23505	Pt	1	0	0.00000
HETATM	81	Pt	6.44603	11.16485	18.23503	Pt	1	0	0.00000
HETATM	82	Pt	-0.00003	-0.00004	20.51616	Pt	1	0	0.00000
HETATM	83	Pt	0.00004	2.79121	20.51616	Pt	1	0	0.00000
HETATM	84	Pt	-0.00003	5.58247	20.51616	Pt	1	0	0.00000
HETATM	85	Pt	2.41723	1.39565	20.51616	Pt	1	0	0.00000
HETATM	86	Pt	2.41724	4.18678	20.51616	Pt	1	0	0.00000
HETATM	87	Pt	2.41731	6.97803	20.51616	Pt	1	0	0.00000
HETATM	88	Pt	4.83457	2.79121	20.51616	Pt	1	0	0.00000
HETATM	89	Pt	4.83450	5.58247	20.51616	Pt	1	0	0.00000
HETATM	90	Pt	4.83450	8.37360	20.51616	Pt	1	0	0.00000
HETATM	91	Pt	0.80545	1.39508	22.79717	Pt	1	0	0.00000
HETATM	92	Pt	0.80545	4.18734	22.79717	Pt	1	0	0.00000
HETATM	93	Pt	0.80635	6.97803	22.79717	Pt	1	0	0.00000
HETATM	94	Pt	3.22362	2.79121	22.79717	Pt	1	0	0.00000
HETATM	95	Pt	3.22271	5.58190	22.79717	Pt	1	0	0.00000
HETATM	96	Pt	3.22271	8.37416	22.79717	Pt	1	0	0.00000
HETATM	97	Pt	5.63997	4.18734	22.79717	Pt	1	0	0.00000
HETATM	98	Pt	5.64088	6.97803	22.79717	Pt	1	0	0.00000
HETATM	99	Pt	5.63997	9.76872	22.79717	Pt	1	0	0.00000
HETATM	100	Pt	1.61151	2.79121	25.07396	Pt	1	0	0.00000
HETATM	101	Pt	1.61151	5.58242	25.08019	Pt	1	0	0.00000
HETATM	102	Pt	1.61151	8.37364	25.08019	Pt	1	0	0.00000
HETATM	103	Pt	4.02877	4.18682	25.08019	Pt	1	0	0.00000
HETATM	104	Pt	4.02877	6.97803	25.07396	Pt	1	0	0.00000
HETATM	105	Pt	4.02877	9.76924	25.08019	Pt	1	0	0.00000
HETATM	106	Pt	6.44603	5.58242	25.08019	Pt	1	0	0.00000
HETATM	107	Pt	6.44603	8.37364	25.08019	Pt	1	0	0.00000
HETATM	108	Pt	6.44603	11.16485	25.07396	Pt	1	0	0.00000
HETATM	109	Pt	-0.00493	-0.00854	27.35859	Pt	1	0	0.00000
HETATM	110	Pt	0.00985	2.79121	27.35859	Pt	1	0	0.00000
HETATM	111	Pt	-0.00493	5.59096	27.35859	Pt	1	0	0.00000
HETATM	112	Pt	2.41233	1.40414	27.35859	Pt	1	0	0.00000
HETATM	113	Pt	2.41233	4.17828	27.35859	Pt	1	0	0.00000
HETATM	114	Pt	2.42711	6.97803	27.35859	Pt	1	0	0.00000
HETATM	115	Pt	4.84437	2.79121	27.35859	Pt	1	0	0.00000
HETATM	116	Pt	4.82959	5.59096	27.35859	Pt	1	0	0.00000
HETATM	117	Pt	4.82959	8.36510	27.35859	Pt	1	0	0.00000
HETATM	118	Pt	0.81499	1.41161	29.72128	Pt	1	0	0.00000
HETATM	119	Pt	0.81499	4.17081	29.72128	Pt	1	0	0.00000
HETATM	120	Pt	0.78727	6.97803	29.72128	Pt	1	0	0.00000
HETATM	121	Pt	3.20453	2.79121	29.72128	Pt	1	0	0.00000
HETATM	122	Pt	3.23225	5.59843	29.72128	Pt	1	0	0.00000
HETATM	123	Pt	3.23225	8.35763	29.72128	Pt	1	0	0.00000
HETATM	124	Pt	5.64951	4.17081	29.72128	Pt	1	0	0.00000
HETATM	125	Pt	5.62179	6.97803	29.72128	Pt	1	0	0.00000
HETATM	126	Pt	5.64951	9.78525	29.72128	Pt	1	0	0.00000
HETATM	127	O	1.61151	2.79121	30.84302	O	1	0	0.00000
HETATM	128	O	1.61151	2.79121	-1.21582	O	1	0	0.00000
HETATM	129	O	4.02877	6.97803	30.84302	O	1	0	0.00000
HETATM	130	O	6.44603	11.16485	30.84302	O	1	0	0.00000
HETATM	131	O	4.02877	6.97803	-1.21582	O	1	0	0.00000
HETATM	132	O	6.44603	11.16485	-1.21582	O	1	0	0.00000

UNIT ENERGY kcal
ENERGY -16995.842213
END

XTLGRF 200
DESCRP A0088
REMARK Pt111_0.50ML_2x1x14_30.0_vac
RUTYPE NORMAL RUN
FIXATOMS 13 16
CRYSTX 5.58242 2.79121 59.62720 90.00000 90.00000 60.00000

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HETATM 1 Pt 0.00128 0.00000 -0.03099 Pt 1 0 0.00000
HETATM 2 Pt 2.37566 1.39561 -0.32773 Pt 1 0 0.00000
HETATM 3 Pt 0.81388 1.39561 2.23856 Pt 1 0 0.00000
HETATM 4 Pt 3.20649 2.79121 2.30691 Pt 1 0 0.00000
HETATM 5 Pt 1.59949 2.79121 4.55034 Pt 1 0 0.00000
HETATM 6 Pt 4.02719 4.18682 4.55832 Pt 1 0 0.00000
HETATM 7 Pt -0.00344 0.00000 6.83632 Pt 1 0 0.00000
HETATM 8 Pt 2.41270 1.39561 6.83179 Pt 1 0 0.00000
HETATM 9 Pt 0.80543 1.39561 9.11455 Pt 1 0 0.00000
HETATM 10 Pt 3.22206 2.79121 9.11335 Pt 1 0 0.00000
HETATM 11 Pt 1.61236 2.79121 11.39418 Pt 1 0 0.00000
HETATM 12 Pt 4.02944 4.18682 11.39378 Pt 1 0 0.00000
HETATM 13 Pt 0.00000 0.00000 13.67409 Pt 1 0 0.00000
HETATM 14 Pt 2.41726 1.39561 13.67409 Pt 1 0 0.00000
HETATM 15 Pt 0.80575 1.39561 15.95311 Pt 1 0 0.00000
HETATM 16 Pt 3.22301 2.79121 15.95311 Pt 1 0 0.00000
HETATM 17 Pt 1.61065 2.79121 18.23302 Pt 1 0 0.00000
HETATM 18 Pt 4.02809 4.18682 18.23342 Pt 1 0 0.00000
HETATM 19 Pt 0.00095 0.00000 20.51385 Pt 1 0 0.00000
HETATM 20 Pt 2.41758 1.39561 20.51265 Pt 1 0 0.00000
HETATM 21 Pt 0.81031 1.39561 22.79541 Pt 1 0 0.00000
HETATM 22 Pt 3.22645 2.79121 22.79088 Pt 1 0 0.00000
HETATM 23 Pt 1.62352 2.79121 25.07686 Pt 1 0 0.00000
HETATM 24 Pt 4.03034 4.18682 25.06888 Pt 1 0 0.00000
HETATM 25 Pt 0.01652 0.00000 27.32029 Pt 1 0 0.00000
HETATM 26 Pt 2.40913 1.39561 27.38864 Pt 1 0 0.00000
HETATM 27 Pt 0.84735 1.39561 29.95493 Pt 1 0 0.00000
HETATM 28 Pt 3.22173 2.79121 29.65819 Pt 1 0 0.00000
HETATM 29 O 1.82724 2.79121 30.96101 O 1 0 0.00000
HETATM 30 O 1.39577 2.79121 -1.33381 O 1 0 0.00000
UNIT ENERGY kcal
ENERGY -3825.367178
END

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XTLGRF 200
DESCRP A0099
REMARK Pt111_0.75ML_4x1x12_30.0_vac
RUTYPE NORMAL RUN
FIXATOMS 21 28
CRYSTX 11.16485 2.79121 55.06917 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 0.00153 0.00002 0.04219 Pt 1 0 0.00000
HETATM 2 Pt 2.42809 1.39560 -0.03397 Pt 1 0 0.00000
HETATM 3 Pt 4.84425 2.79122 -0.00365 Pt 1 0 0.00000
HETATM 4 Pt 7.24087 4.18688 -0.00726 Pt 1 0 0.00000
HETATM 5 Pt 0.81426 1.39557 2.29064 Pt 1 0 0.00000
HETATM 6 Pt 3.22195 2.79116 2.26491 Pt 1 0 0.00000
HETATM 7 Pt 5.63941 4.18677 2.27973 Pt 1 0 0.00000
HETATM 8 Pt 8.05416 5.58239 2.28420 Pt 1 0 0.00000
HETATM 9 Pt 1.61389 2.79112 4.56164 Pt 1 0 0.00000
HETATM 10 Pt 4.02675 4.18672 4.55194 Pt 1 0 0.00000
HETATM 11 Pt 6.44508 5.58234 4.55987 Pt 1 0 0.00000
HETATM 12 Pt 8.86365 6.97795 4.56140 Pt 1 0 0.00000
HETATM 13 Pt 0.00019 -0.00010 6.83913 Pt 1 0 0.00000
HETATM 14 Pt 2.41774 1.39550 6.83774 Pt 1 0 0.00000
HETATM 15 Pt 4.83324 2.79110 6.83460 Pt 1 0 0.00000
HETATM 16 Pt 7.25141 4.18672 6.83869 Pt 1 0 0.00000
HETATM 17 Pt 0.80614 1.39554 9.11687 Pt 1 0 0.00000
HETATM 18 Pt 3.22318 2.79115 9.11595 Pt 1 0 0.00000
HETATM 19 Pt 5.63969 4.18675 9.11540 Pt 1 0 0.00000
HETATM 20 Pt 8.05754 5.58237 9.11715 Pt 1 0 0.00000
HETATM 21 Pt 1.61151 2.79121 11.39508 Pt 1 0 0.00000

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HETATM	22	Pt	4.02877	4.18682	11.39508	Pt	1	0	0.00000
HETATM	23	Pt	6.44603	5.58242	11.39508	Pt	1	0	0.00000
HETATM	24	Pt	8.86329	6.97803	11.39508	Pt	1	0	0.00000
HETATM	25	Pt	0.00000	0.00000	13.67409	Pt	1	0	0.00000
HETATM	26	Pt	2.41726	1.39561	13.67409	Pt	1	0	0.00000
HETATM	27	Pt	4.83452	2.79121	13.67409	Pt	1	0	0.00000
HETATM	28	Pt	7.25178	4.18682	13.67409	Pt	1	0	0.00000
HETATM	29	Pt	0.80664	1.39561	15.95387	Pt	1	0	0.00000
HETATM	30	Pt	3.22340	2.79121	15.95164	Pt	1	0	0.00000
HETATM	31	Pt	5.64158	4.18682	15.95262	Pt	1	0	0.00000
HETATM	32	Pt	8.05906	5.58242	15.95415	Pt	1	0	0.00000
HETATM	33	Pt	1.61265	2.79121	18.23303	Pt	1	0	0.00000
HETATM	34	Pt	4.02879	4.18682	18.22814	Pt	1	0	0.00000
HETATM	35	Pt	6.44810	5.58242	18.23206	Pt	1	0	0.00000
HETATM	36	Pt	8.86547	6.97803	18.23483	Pt	1	0	0.00000
HETATM	37	Pt	0.00262	-0.00000	20.51596	Pt	1	0	0.00000
HETATM	38	Pt	2.41759	1.39560	20.51226	Pt	1	0	0.00000
HETATM	39	Pt	4.83302	2.79121	20.50291	Pt	1	0	0.00000
HETATM	40	Pt	7.25477	4.18682	20.51321	Pt	1	0	0.00000
HETATM	41	Pt	0.80719	1.39560	22.79908	Pt	1	0	0.00000
HETATM	42	Pt	3.22295	2.79121	22.78989	Pt	1	0	0.00000
HETATM	43	Pt	5.63438	4.18682	22.77384	Pt	1	0	0.00000
HETATM	44	Pt	8.06519	5.58242	22.79774	Pt	1	0	0.00000
HETATM	45	Pt	1.61940	2.79121	25.07494	Pt	1	0	0.00000
HETATM	46	Pt	4.01540	4.18681	25.07581	Pt	1	0	0.00000
HETATM	47	Pt	6.44178	5.58242	25.02761	Pt	1	0	0.00000
HETATM	48	Pt	8.87365	6.97803	25.10441	Pt	1	0	0.00000
HETATM	49	Pt	0.28726	-0.00000	27.65559	Pt	1	0	0.00000
HETATM	50	Pt	4.73811	2.79121	27.44732	Pt	1	0	0.00000
HETATM	51	Pt	7.39627	4.18682	27.48425	Pt	1	0	0.00000
HETATM	52	Pt	2.60947	1.39560	29.22827	Pt	1	0	0.00000
HETATM	53	O	8.16330	5.58242	28.62788	O	1	0	0.00000
HETATM	54	O	1.19711	2.79121	29.51459	O	1	0	0.00000
HETATM	55	O	4.05975	2.79121	29.35253	O	1	0	0.00000
HETATM	56	Pt	3.51515	2.79117	-2.58653	Pt	1	0	0.00000
HETATM	57	Pt	7.96521	5.58268	-2.37862	Pt	1	0	0.00000
HETATM	58	Pt	10.62354	6.97768	-2.41505	Pt	1	0	0.00000
HETATM	59	Pt	5.83624	4.18703	-4.16124	Pt	1	0	0.00000
HETATM	60	O	1.72177	-0.00007	-3.55851	O	1	0	0.00000
HETATM	61	O	4.42386	2.79134	-4.44619	O	1	0	0.00000
HETATM	62	O	7.28667	5.58268	-4.28383	O	1	0	0.00000

UNIT ENERGY kcal
ENERGY -7788.991477
END

XTLGRF 200
DESCRP A0066
REMARK Pt111_1.00ML_4x1x12_30.0_vac
FIXATOMS 21 28
CRYSTX 11.16482 2.79121 55.06910 90.00000 90.00000 60.00000
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HETATM	2	Pt	2.33516	1.39560	-0.30543	Pt	1	0	0.00000
HETATM	3	Pt	4.91013	2.79121	0.03774	Pt	1	0	0.00000
HETATM	4	Pt	7.24527	4.18681	-0.05108	Pt	1	0	0.00000
HETATM	5	Pt	0.77422	1.39560	2.26346	Pt	1	0	0.00000
HETATM	6	Pt	3.19698	2.79120	2.24166	Pt	1	0	0.00000
HETATM	7	Pt	5.63357	4.18681	2.31257	Pt	1	0	0.00000
HETATM	8	Pt	8.02600	5.58241	2.26751	Pt	1	0	0.00000
HETATM	9	Pt	1.59119	2.79121	4.54167	Pt	1	0	0.00000
HETATM	10	Pt	4.00394	4.18681	4.54621	Pt	1	0	0.00000
HETATM	11	Pt	6.43101	5.58241	4.57277	Pt	1	0	0.00000
HETATM	12	Pt	8.84289	6.97801	4.54905	Pt	1	0	0.00000

HETATM	13	Pt	-0.01385	-0.00000	6.82970	Pt	1	0	0.00000
HETATM	14	Pt	2.40117	1.39560	6.82804	Pt	1	0	0.00000
HETATM	15	Pt	4.81783	2.79120	6.83332	Pt	1	0	0.00000
HETATM	16	Pt	7.24016	4.18680	6.84174	Pt	1	0	0.00000
HETATM	17	Pt	0.79819	1.39560	9.11222	Pt	1	0	0.00000
HETATM	18	Pt	3.21424	2.79120	9.11244	Pt	1	0	0.00000
HETATM	19	Pt	5.63198	4.18681	9.11496	Pt	1	0	0.00000
HETATM	20	Pt	8.05128	5.58241	9.11677	Pt	1	0	0.00000
HETATM	21	Pt	1.61150	2.79121	11.39505	Pt	1	0	0.00000
HETATM	22	Pt	4.02876	4.18681	11.39505	Pt	1	0	0.00000
HETATM	23	Pt	6.44601	5.58241	11.39505	Pt	1	0	0.00000
HETATM	24	Pt	8.86327	6.97801	11.39505	Pt	1	0	0.00000
HETATM	25	Pt	0.00000	0.00000	13.67406	Pt	1	0	0.00000
HETATM	26	Pt	2.41725	1.39560	13.67406	Pt	1	0	0.00000
HETATM	27	Pt	4.83451	2.79121	13.67406	Pt	1	0	0.00000
HETATM	28	Pt	7.25176	4.18681	13.67406	Pt	1	0	0.00000
HETATM	29	Pt	0.80692	1.39560	15.95582	Pt	1	0	0.00000
HETATM	30	Pt	3.22383	2.79120	15.95308	Pt	1	0	0.00000
HETATM	31	Pt	5.64275	4.18681	15.95419	Pt	1	0	0.00000
HETATM	32	Pt	8.06109	5.58241	15.95814	Pt	1	0	0.00000
HETATM	33	Pt	1.61204	2.79121	18.23578	Pt	1	0	0.00000
HETATM	34	Pt	4.03057	4.18681	18.23012	Pt	1	0	0.00000
HETATM	35	Pt	6.45297	5.58241	18.23475	Pt	1	0	0.00000
HETATM	36	Pt	8.86970	6.97802	18.24537	Pt	1	0	0.00000
HETATM	37	Pt	0.00482	0.00000	20.53816	Pt	1	0	0.00000
HETATM	38	Pt	2.41323	1.39561	20.50937	Pt	1	0	0.00000
HETATM	39	Pt	4.84651	2.79121	20.50063	Pt	1	0	0.00000
HETATM	40	Pt	7.26046	4.18681	20.52231	Pt	1	0	0.00000
HETATM	41	Pt	0.78827	1.39561	22.84087	Pt	1	0	0.00000
HETATM	42	Pt	3.26032	2.79121	22.74414	Pt	1	0	0.00000
HETATM	43	Pt	5.64907	4.18681	22.79623	Pt	1	0	0.00000
HETATM	44	Pt	8.04675	5.58242	22.81742	Pt	1	0	0.00000
HETATM	45	Pt	1.71112	2.79122	25.08693	Pt	1	0	0.00000
HETATM	46	Pt	4.03544	4.18682	25.09108	Pt	1	0	0.00000
HETATM	47	Pt	6.38478	5.58242	25.10351	Pt	1	0	0.00000
HETATM	48	Pt	8.75629	6.97802	25.14942	Pt	1	0	0.00000
HETATM	49	Pt	0.20724	0.00001	28.13340	Pt	1	0	0.00000
HETATM	50	Pt	4.50493	2.79124	27.57221	Pt	1	0	0.00000
HETATM	51	Pt	7.27319	4.18680	27.66068	Pt	1	0	0.00000
HETATM	52	Pt	2.55728	1.39564	29.65935	Pt	1	0	0.00000
HETATM	53	O	7.90547	5.58242	28.88142	O	1	0	0.00000
HETATM	54	O	1.16743	2.79124	30.02334	O	1	0	0.00000
HETATM	55	O	3.99818	2.79124	29.59397	O	1	0	0.00000
HETATM	56	O	0.86714	2.79124	26.56959	O	1	0	0.00000
HETATM	57	Pt	1.77879	2.79120	-2.99853	Pt			